Terahertz bound states in the continuum

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TERAHERTZ BOUND STATES IN THE CONTINUUM

HAN SONG

SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

2020

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HAN SONG

SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

A thesis submitted to the Nanyang Technological
University in partial fulfilment of the requirement for the
degree of Doctor of Philosophy
2020

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research done by me except where otherwise stated in this thesis. The thesis work has not been submitted for a degree or professional qualification to any other university or institution. I declare that this thesis is written by myself and is free of plagiarism and of sufficient grammatical clarity to be examined. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

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Authorship Attribution Statement

This thesis contains material from 1 paper(s) published in the following peer-reviewed journal(s) / from papers accepted at conferences in which I am listed as an author.

Chapter 3 is published as S. Han, L. Cong, Y. K. Srivastava, B. Qiang, M. V. Rybin, A. Kumar, R. Jain, W. X. Lim, V. G. Achanta, S. S. Prabhu, Q. J. Wang, Y. S. Kivshar, and R. Singh. All-Dielectric Active Terahertz Photonics Driven by Bound States in the Continuum, *Adv. Mater.* 31(37), 1901921 (2019). DOI: 10.1002/adma.201901921.

The contributions of the co-authors are as follows:

- Assoc/Prof Singh provided the initial project direction. Prof. Singh and Prof. Yuri edited the manuscript drafts.
- I prepared the manuscript drafts. The manuscript was revised by Dr. Cong and Dr. Rybin.
- The sample fabrications (UV lithography) were conducted by Dr. Srivastava and me in the Clean Room 2 at electric and electronic engineering, Nanyang Technological University. Dr. Gang Yih Chong was helping to performing reactive ion etching and deep reactive ion etching.
- With Dr. Longqing's assistance, I designed the study and performed all the laboratory work at the ultrafast terahertz photonics lab in center for disruptive photonic technologies (CDPT) at School of Physical and Mathematical Sciences, Nanyang Technological University. I also analyzed the data.
- In addition, Mr. A. Kumar helped to measure the highest Q -factor sample with Mr. R. Jain at the group at Tata Institute of Fundamental Research, India.
- All simulations were done by me and Qiang Bo. The theoretical analysis was done by Dr. Rybin and me.
- Dr. Lim assisted in the taking SEM images.

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- All simulations were done by me. With assistance from Dr. Rybin, the theoretical analysis was done by me.

Note: If published materials are not inserted as thesis chapters, students must acknowledge co-worker contributions in the acknowledgement section of their thesis.

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Abstract

Localized wave confinement in electromagnetic devices is crucial in science and technology. Waves can be confined with diverse methods ranging from metallic reflectors, total internal reflection, photonic bandgap, to Anderson localization and symmetry separability, where the “resonator” is surrounded by a medium that does not support outgoing waves, which inevitably trapping the waves in it. Recently, it has been found that waves can sometimes be perfectly trapped without leakages through symmetry separability which is known as a bound state in continuum (BIC). It has a localized eigenstate, whose frequency (or energy) lies within the continuous plane waves. In this thesis, we numerically and experimentally investigate diverse resonant all-dielectric metamaterials and photonic crystal (PhC) slabs for observation of these non-radiating BICs. A 2D dielectric metasurface is proposed to demonstrate supercavity govern by the BICs under TE-polarized excitation. With silicon as the metasurface building blocks, the supercavity enables low-fluence ($10.16 \mu\text{J}/\text{cm}^2$) switching at nanosecond time scales. Under TM-polarized excitations, terahertz guided mode resonances (GMRs) are also discovered in the same 2D dielectric metasurfaces. It is also observed multiple BICs at terahertz regime by employing a C_{4v} symmetric metasurface and their diverse counterparts with in-plane symmetry breaking. The BICs, demonstrated by ultra-high- Q resonances enable extremely high field localization, which are desired for low-threshold terahertz quantum cascade

lasers. Finally, we investigate, for the first time, the dynamic zero-index BICs in terahertz large-scale integrated photonic devices. The zero-index is realized by constructing an accidental degeneracy dispersion, also known as photonic Dirac-like cone, which enables non-radiating BICs such that a low-loss zero-index PhC slab is achieved. The active modulation of zero-index PhC is also demonstrated. This thesis opens up bright avenues for designing low-loss, on-chip, and dynamic terahertz resonant devices.

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Table of Contents

Abstract	1
Acknowledgements.....	3
Table of Contents	5
List of Figures.....	8
 Chapter 1: Introduction	 10
1.1 Towards filling the “Terahertz Gap”	10
1.2 Photonic crystals	13
1.2.1 All-dielectric resonant photonic crystals.....	15
1.2.2 Exploring zero-linewidth resonances	18
1.3 Active photonic metamaterials and terahertz wave modulation	20
1.4 Organization of the thesis.....	23
 Chapter 2: Rigorous coupled wave analysis for periodic gratings.....	 26
2.1 Background.....	26
2.2 Single layer gratings.....	27
2.2.1 Permittivity expansion for binary gratings.....	27
2.2.2 TE-polarized incidence.....	29
2.2.3 TM-polarized incidence.....	36
2.3 Multilayer binary gratings	39
2.4 2D gratings	47
2.5 Conclusion.....	52
 Chapter 3: All-dielectric active photonics driven by bound states in the continuum.....	 53
3.1 Introduction	53
3.2 Bound states in the continuum and supercavity modes.....	54
3.3.1 Numerical simulation	57

3.3.2	Numerical results.....	58
3.3.3	Parameter optimization.....	62
3.4	Experimental observation of terahertz supercavity modes	64
3.4.1	Sample fabrication.....	64
3.4.2	Materials characterization with THz-TDS.....	66
3.4.3	CW Terahertz spectroscopy	67
3.4.4	Experimental results	68
3.5	Active control of terahertz supercavity modes	70
3.5.1	ZnTe-based optical-pump terahertz probe spectroscopy	70
3.5.2	Dynamic supercavity modulations	71
3.5.3	Pump fluence dependent dynamics and transmission spectra.....	75
3.6	Conclusion.....	76
Chapter 4: Guided-mode resonances in dielectric terahertz metasurfaces		78
4.1	Introduction	78
4.2	Guided-mode resonances.....	79
4.3	Metasurface building blocks and experimental measurements.....	80
4.4	Additional measurements	87
4.5	Localized field enhanced by symmetry-protected bound states in the continuum.....	87
4.6	Parameter optimization.....	89
4.7	Conclusion.....	91
Chapter 5: In-plane symmetry breaking induced terahertz bound states in the continuum		93
5.1	Introduction	93
5.2	Bound states in the continuum in C_{4v} photonic lattice.....	95
5.3	In-plane C_{4v} symmetry breaking	98
5.4	Fabrication and measurement	102
5.5	Experimental observation of terahertz quasi-BICs	103
5.6	conclusion.....	106

Chapter 6: Dynamic bound states in the continuum in zero-index photonic crystal slab	107
6.1 Introduction	107
6.2 Design and fabrication.....	109
6.3 Point-group symmetry analysis.....	110
6.4 Zero-index on photonic Dirac cone.....	113
6.5 Terahertz angle-resolved time-domain measurements.....	115
6.5.1 TE-polarized far field terahertz measurements	115
6.5.2 Dynamic zero-index PhC.....	117
6.5.3 Experimental proposal for measuring zero-index bound states in the continuu.....	118
6.6 Conclusion	119
Chapter 7: Conclusion and outlooks.....	120
7.1 Conclusion.....	120
7.2 Outlooks	121
Appendix I: Publication list	123
Bibliography	125

List of Figures

Figure 1-1. The terahertz “gap”	11
Figure 1-2. A snapshot of the unique applications in the terahertz regime.....	13
Figure 1-3. One-, two-, and three-dimensional photonic crystals	14
Figure 1-4. TE- and TM-polarized band structures and field profiles for 1D silicon binary grating.....	15
Figure 1-5. TE- and TM-polarized transmission of 1D silicon grating.....	17
Figure 1-6. A single resonance for optical BICs in a photonic crystal slab	19
Figure 2-1. Schematic view of single-layer binary grating	28
Figure 2-2. Study single-layer binary grating with TE-polarized RCWA algorithm.....	35
Figure 2-3. Excitation of BIC in 1D binary grating with TM-polarized plane wave	39
Figure 2-4. Discovery Dirac-cone dispersion in multilayered 1D gratings	42
Figure 2-5. Field profile of the multilayer gratings for TE-/TM-polarizations	46
Figure 2-6. Schematic representation of a 2D grating.....	47
Figure 3-1. Metasurface design for THz supercavity with extreme high- Q resonances.....	56
Figure 3-2. BICs and supercavity resonance.....	60
Figure 3-3. The transmission map as function of the resonator width	62
Figure 3-4. The transmission map as function of the resonator height	64
Figure 3-5. Experimental study the terahertz properties of 200 μm Si and 1 mm quartz	67
Figure 3-6. Experimental measurement	69
Figure 3-7. Dynamic supercavity modulation.....	73
Figure 3-8. Temporal evolution of the supercavity	74
Figure 3-9. The dynamic evolution and corresponding transmission spectra of optically pumped device under different fluences	76
Figure 4-1. Terahertz metasurface design for exciting GMRs.....	81
Figure 4-2. Simulations and measurements	84

Figure 4-3. Additional experiments	87
Figure 4-4. Terahertz GMRs near the Γ point.....	89
Figure 4-5. Parameter engineering for experimental terahertz GMRs	90
Figure 5-1. Theoretical predictions of C_{4v} symmetric dielectric metasurface	96
Figure 5-2. In-plane symmetry breaking	100
Figure 5-3. Two additional methods for in-plane symmetry breakings	101
Figure 5-4. Fabricated samples and fiber-based THz-TDs measurement.....	103
Figure 5-5. Experimental measurements of the quasi-BICs by varying d_x	104
Figure 5-6. Experimental measurements of the quasi-BICs by varying d_y	105
Figure 6-1. Design of terahertz “daisy” PhC slab.....	110
Figure 6-2. Eigenmode analysis.....	112
Figure 6-3. Zero-index analysis	114
Figure 6-4. Experimental measurements on three fabricated samples	116
Figure 6-5. Numerical simulations and experimental measurements.....	116
Figure 6-6. Active control of PhC modes with OTP	118
Figure 6-7. $Re\{E_z\}$ for a triangular zero-index PhC region surrounded by uniform silicon slab	119

Chapter 1: Introduction

1.1 Towards filling the “Terahertz Gap”

The terahertz spectrum extends from 10^{11} - 10^{13} Hz (0.1 - 10 THz) that lies between the microwave and infrared regions of the electromagnetic (EM) spectrum, as shown in **Figure 1-1(a)**. Terahertz region therefore falls in between the electronic-dominated and photonic-dominated realms of the EM spectrum. The realization of terahertz technology is largely lacking due to unavailability of efficient terahertz sources, detectors and functional components. Therefore, it was termed as a “terahertz gap” for a long time [1-4]. The main challenges for constructing suitable terahertz sources are the microwave electronics exhibit lower output power with increasing frequency, and the output power of optical photonic sources also exhibits decreasing trend with decreasing frequency, as shown in **Figure 1-1(b)** [4]. The advent of mode-locked femtosecond lasers in early 1990s have enabled the development of terahertz time-domain spectroscopy (THz-TDS), where terahertz radiation is generated by optical pumping of photoactive antennas made of semiconductors (GaAs, GaP, et al.), or using optical rectification of nonlinear crystals (ZnTe, DAST, and LiNbO₃, et al.) [4-17]. Significant advancements have been made in terms of achieving extremely large bandwidth and high-power terahertz sources. Optical rectification in ZnSe and GaP, organic crystals, and more recently the optically driven spin currents in multilayer materials have been employed to generate extremely broadband terahertz generation [10, 16, 18-24]. Titled-pulse-front pumping of LiNbO₃, optical rectification in organic crystals, air and/or gases-plasma and relativistic laser-plasma have been utilized to generate intense terahertz beams [10, 16, 25-27]. InGaAs-based photomixers excited by distributed feedback (DFB) lasers have been recently commercialized for continuous-wave (CW) terahertz spectroscopy [28]. Terahertz quantum cascade lasers (QCLs) have also been well developed for deliver 100 milliwatts or more of CW coherent radiation [9, 12].

Figure 1-1. The terahertz “gap”—(a) Terahertz regime of the EM spectrum. (b) Terahertz regime is considered as a frequency gap in the EM spectrum that is mainly illustrated by the emission power [4]. *Solid lines* stand for conventional sources and *oval shapes* demonstrate recent terahertz sources. IMPATT (i.e. impact ionization avalanche transit-time diode), MMIC (i.e. microwave monolithic integrated circuit), TUNNET (i.e. tunnel injection transit time), UTC-PD (i.e. uni-traveling-carrier photodiode), DFG (i.e. difference frequency generator) and QCL (i.e. quantum cascade laser) are labelled as abbreviations, and multiplexer is a Schottky barrier diode (SBD) frequency multiplier.

With the stabilized and high-efficiency terahertz to be generated and the corresponding suitable detection technologies, vast range of fundamental researches and applications gathered in terahertz region, as shown in **Figure 1-2**. For physics and materials science, terahertz spectroscopy has been employed to visualize spectral features related fundamental physics, such as vibrational motion of organic compounds, phonon resonances (lattice vibrations) in solids, energy gaps of superconductors, intra-band transitions and carrier dynamics in semiconductors, and rotational transitions of molecules [1-17, 29, 30]. Intense terahertz radiation is promising for high harmonic generation in condensed matter systems, resonant and non-resonant manipulations of materials, and charged particle accelerations [10, 16, 29, 30]. For information and communications, electronics and photonics accelerated terahertz technologies are expected to meet the ever-increasing demand for high-capacity and high-speed wireless communications [31, 32]. Owing to the stark contrasts of different media in terahertz band, many imaging applications ranging from basic scientific missions to commercial projects are possible, such as nondestructive testing for sealed packages, security applications and medical applications [4-6, 14-17, 33-41]. In security, terahertz radiation can penetrate through the package that is usually made of dielectrics and detect the metallic inclusions [37]. It is easy to differentiate the hydrated substances from dried ones due to the high absorption of terahertz waves by water molecules [38]. In biology, the molecular dynamics associating with vibrational motions and inter molecular interactions can be monitored from the spectral signatures by terahertz spectroscopy due to its non-ionizing and non-destructive features [39-41]. The harmless detection of explosives and illicit drugs, testing of pharmaceutical products and protein conformation, are also feasible by terahertz spectroscopy [42]. In medical applications, the sensitivity of water in terahertz spectrum would provide the useful tool to inspect the water content that is crucial for the quality of drugs and biological systems [38, 42].

Figure 1-2. A snapshot of the unique applications in the terahertz regime [38].

1.2 Photonic crystals

Photonic crystals (PhCs) are artificially structured EM media with periodically modulated EM parameters. Their EM properties can be analogue to the electronic eigenmodes of condensed matter with periodically tailored electronic potentials. Therefore, the EM waves in the PhCs and their dispersion relations (or band structures) can be computed by solving the Maxwell eigenequations from the well-known Bloch-Floquet theorem [43-46]. Besides the photonic band structures, i.e. propagating eigenmodes, another distinct characteristic for the PhCs is their photonic band gaps that prevent the EM waves from propagating through the photonic structure. In 1887 L. Rayleigh firstly studied EM wave propagation in periodic multi-layer dielectric stacks that show photonic band gap in one dimension [47]. Due to the prohibiting propagation of band gap, their experiments observed reflective properties of their 2D PhCs. This reflectivity is angle-dependent, due to the differing periodicities experienced by light propagating at different angles of incidence. Although such multilayer films received intensive

study interests over the following century, no one used the term *photonic crystal* until 100 years later. In 1987, E. Yablonovitch and S. John joined the tools of classical electromagnetism and solid-state physics to introduce the concept of omnidirectional photonic band gaps in two-, and three-dimensions (or, 1D, 2D, and 3D) [46]. This extended the PhCs to be classified as one-, two-, and three-dimensional according to their periodicities along different axis, as shown in **Figure 1-3**. The 1D PhC is a stack of periodically alternative layers of materials with different dielectric parameters. It is periodic only in y -axis, but uniform in x -, and z -axis. For a 2D PhC, the periodicities are along x -, and y -axis, while it is uniform along z -axis. 2D PhCs can be truncated at z -axis to form a slab cladded by contrast materials that is known as PhC slabs. In 3D PhCs, the dielectric parameters are periodically modulated in all x -, y -, and z -directions.

Figure 1-3. Classification of one-, two-, and three-dimensional photonic crystals [46].

Recent years, the developments in their fabrication and theory allow the PhCs to be applied to various purposes [48], such as lasing, sensing, wavelength multiplexing, photonic topological insulators, and other telecommunication applications. These applications are based on several interesting properties of the photonic band structure and on their particular dispersion, e.g., modification of spontaneous emission or birefringence, super-prism effect and negative refraction [49]. Photonic waveguides with modes below light line are one of the most important

components in photonic integrated circuits, as they connect the different functional elements, such as sources, modulators, multiplexers, or detectors [50]. Moreover, the photonic modes above the light cone also draw many research interests due to their capability of leakage, i.e. coupling to the free space [51]. Next, we'll analyze these eigenmodes by employing simple 1D silicon grating.

1.2.1 All-dielectric resonant photonic crystals

Figure 1-4 shows the TE and TM band structures and their respective (electric and magnetic) field profiles of 1D silicon grating suspended in air. The band nomenclature is characterized by each irreducible representation of group theory, where the grating presented here belongs to the D_{2h} point group with given symmetric operations [52].

Figure 1-4. TE- and TM-polarized band structures and field profiles for 1D silicon binary grating. The grating has period $\Lambda = 300 \mu\text{m}$, grating width $W = 150 \mu\text{m}$, grating thickness $t = 150 \mu\text{m}$, grating permittivity $\epsilon_g = 11.9$, and air permittivity $\epsilon_a = 1$. (a) TE dispersion and (b) TM dispersion.

In general, the solved band structures of this binary grating can be classified into three regions. The first region is the modes that lie below the light cone (white region), where no state is allowed outside the grating. These modes will be guided through total internal reflection (TIR) at the interface between the grating and superstrate and substrate (air) claddings. Therefore, they are pure lossless Bloch modes. The fundamental guided mode has no cutoff frequency and always lies below the light line if the grating is symmetrically cladded. Consequently, the system supports at least one guided mode. However, an asymmetrical cladding (for example, the presence of substrate) may be introduced to the actual devices, which break the vertical mirror symmetry. This leads to a finite cutoff frequency for the fundamental mode. The cutoff frequency increases with increasing asymmetry [53]. Therefore, it is possible that the lowest mode lies entirely above the light line, and no guided mode exists for such systems. These modes lie above the light cone (radiation continuum) indicated by the gray region in **Figure 1-4** can readily radiate them to free space. Therefore, they have intrinsic radiation losses due to out-of-plane diffraction, hence are also known as resonances or quasi-guided modes [51, 53]. General speaking, the quality (Q) factor, given by $Q = \tau\omega_0/2$, where τ is the lifetime of a resonance and ω_0 is central frequency of resonance, evaluates the coupling strength between resonance mode and free space. The lifetime (τ) of a resonance can be very long (weak radiation losses, high- Q factor) so that the waves get trapped in the system for many cycles before escape. On the contrary, lifetime τ can be very short (strong radiation losses, low- Q factor), as shown in **Figure 1-5**. The radiation losses of resonant modes are related to the index contrast between the grating and the claddings. Enhancement of light localization in PhC slabs and metasurfaces has led to experimental observations of exotic physics phenomena in both fundamental and applied research. This is typically achieved by engineering high- Q factor cavities, where the photons are trapped in the cavities for longer time. Therefore, strong light-

matter interactions can be achieved for many fascinating applications [45-50], such as low-threshold lasing, high harmonic generation, and advanced bio-/chemical sensing.

Figure 1-5. TE- and TM-polarized transmission of 1D silicon binary grating with same geometric and dielectric parameters as **Figure 1-4**. The angle of incidence is zero, and the diffraction channel is indicated by the vertical cyan line at 1 THz.

The third region of the band structure is diffraction modes that is govern by grating law $\sin\theta_m + \sin\theta_i = m\lambda/\Lambda$, where Λ is the grating period, λ is the wavelength, θ_m and θ_i are the angles between the diffracted and incident wave directions, m is an integer representing the diffraction order [47, 54-57]. The diffractions happen only for periodic modulation equal to or larger than the wavelength scale, where the spectral properties rely on the fact that the light impinging on the periodically modulated surface is reflected and/or transmitted at specific angles, as shown in **Figure 1-5**. Thus, the PhCs and metamaterials operating in this region can be used as monochromators, spectrometers, wavelength division multiplexing devices, lasers, chaired pulses amplification, and dielectric laser accelerations [45-50].

1.2.2 Exploring zero-linewidth resonances

Once mathematically predicted by von Neumann and Wigner in quantum mechanics [58], the existence of bound states in the continuum (BICs) has been extensively explored in various physical systems including quantum systems, acoustic and water waves, mathematics, and photonics [58-76]. Two main features can be recognized for the BICs: the mode should be discrete and spatially bound (infinite lifetime or infinite Q -factor), and it also should stay in the radiation continuum (above light cone of photonics), as shown in **Figure 1-6(a)**. Even the leaky mode sometimes shows high- Q and locates at the radiation continuum, it decays quickly since its coupling to the free space. Until recently, the PhC slabs and metamaterials have been proved to be the ideal platform for studying BICs due to their arbitrary building block and size-dependent frequency tunability [77-100]. One of the examples is shown in **Figures 1-6(b)** [82]. The experimental samples were fabricated by drilling air holes on silicon nitride (Si_3N_4) slab, where the Si_3N_4 was grown by low-pressure chemical vapor deposition on silicon dioxide-silicon (SOS) wafer. Angle-resolved spectroscopy was employed to measure the reflections. To avoid mirror symmetry breaking, the superstrate side was immersed in an optical liquid to match the refractive indexes of superstrate and substrate. Two categories of BICs can be differentiated [77, 81, 82, 90], as shown in **Figures 1-6(c)** and **1-6(d)**. The first category is symmetry-protected BICs at Γ point where the coupling to free space is forbidden due to the symmetry mismatch between the systematic mode profile and the external propagating modes (radiation continuum). While away from the Γ point, these states start to be leaky, i.e. coupling to the radiation, since they are no longer protected symmetry. The second one is off- Γ (accidental) BICs, that are unprotected by symmetry and can occur at any unpredicted angle of incidence. Both BICs draw physics interests recently due to its topological nature [90]. The polarization around the BIC is a vortex (2π phase) such that topological charge is well defined [90-93]. In fact, the underlying physics for the second BICs can be simply understood as in-

plane waveguiding and out-of-plane destructive interference since the incident wavevector is projected to k_x and k_z . Therefore, the PhC slab supports guided mode for projected k_x and propagating cancellation (destructive interference) for projected k_z where the radiation is therefore vanished [77, 81, 82].

Figure 1-6. A single resonance for optical BICs in a PhC slab. (a) Illustration and experimental observation of BICs [77]. (b) A schematic illustration of the system. (c) The photonic band structures. (d) The leaky resonance turns into symmetry-protected BICs at Γ point, i.e.

wavevector $k_x a/2\pi = 0$, and off- Γ (or accidental) BICs at wavevector $k_x a/2\pi = 0.25$ (red dots). The radiative Q -factor, Q_r , diverges to infinity at the two BIC regions, as shown by the experimental data (red crosses) and theory (blue line) in (c) [77, 82].

The BICs mode in PhCs and metamaterials provide enhanced mode localization that has enabled many real-world applications [77]. EM field is tightly confined inside the nonlinear materials for building blocks that may enable high-efficiency harmonic generations [94]. Recent studies on metasurfaces have demonstrated high-order (till 9th order) harmonic generations (HHGs) [95]. Here, we indicate that BICs is expected to observe even higher order of the HHGs. In addition, BICs in gain materials can be fabricated to demonstrate PhC surface-emitting lasers (PCSELs) operating at room-temperature with CW condition, low threshold and a high output power [96, 97]. BICs also guarantee advanced chemical and biological sensing where the highly resolved frequency (or wavelength) shift of the extremely high- Q resonance is employed to detect the change of surrounding refractive index [98-100]. To sense the chemical and biological materials, the EM field should be localized outside the building blocks (or penetrated to the chemical and biological materials to be sensed) for high resolutions. Moreover, the higher Q -factors enable narrower linewidths, strong field localization, and higher sensitivity that may be possible for single molecule or monolayer. Surface acoustic waves (SAW) have well-known applications on electronic components, such as delay lines, filters, correlators and DC to DC converters. It has recently been shown that SAWs can be piezoelectrically coupled to superconducting quantum interference device (SQUID). Therefore, efficiently filtering SAWs and their fast propagating can be important for SQUID. A BIC allows SAWs to be propagated at a much faster supersonic speed that is favorable for supersonic SAW filter [101, 102].

1.3 Active photonic metamaterials and terahertz wave modulation

Terahertz wave front modulation, such as amplitude, phase, polarization state, propagation direction, pulse shape and length, plays essential role in terahertz real world applications [103]. Fast and efficient amplitude, phase, and/or polarization modulators are the core technology for high-speed terahertz communication where they are usually employed to encode information in the carrier wave [32]. Spatial encoding terahertz wave front is also the key component in terahertz imaging system where a single sensor in an array of modulators can act as imaging pixels in optical CCD camera [104, 105]. While active modulators are well established as standard devices in optical regime, the high-efficient, ultrafast, and versatile terahertz modulators are still in great demand for the aforementioned applications. Terahertz photonics and metamaterials draw fundamental as well as technological interests for active modulators due to their arbitrary building block, highly compact, and easily integrated characteristics [105]. In general, mechanical, thermal, electric, magnetic, and optical stimulations can be introduced into metamaterials and photonics to realize active modulations.

Thermal actuations can be applied to achieve the structural deformation and phase transition of materials [106-108]. An array of bimorph metamolecules supported by pairs of strips and are designed in a way that bimorph materials sustain different coefficients of thermal expansion [108]. On increasing the ambient temperature, the bimorph strips bend towards the less thermal expansion side and the wave front response is therefore manipulated [108]. Superconductors, for example Yttrium Barium Copper Oxide (YBCO) and Niobium, have been structured as split ring resonators that realize large tunability under thermal or optical stimulus [108-111]. $\text{Ge}_2\text{Sb}_2\text{Te}_5$ (GST) and other phase change materials for metamaterial building blocks possess tunability, where the mechanics is that thermal actuations switch GST from amorphous to crystalline phase [112]. Engagement of the Coulomb force enables the electrically programmable metamaterials controlled by electrical signals. Microelectromechanical systems (MEMS) metamaterial are commonly constructed to work as electrically reconfigurable

metamaterials [108, 112-114]. Similar to the thermal expansion of bimorph structure, the MEMS photonics and metamaterials also contain bimorph reconfiguration, such as Al/Al₂O₃, Au/Si, and Au/SiN_x alloys [112-114]. By applying static electric bias, electrons accumulated at the tips of cantilevers provide the Coulomb repulsive force so that the cantilevers are bent to provide the corresponding spectral response of the metamaterials [114]. The deformation of the cantilevers is positively proportional to the applied electric bias, so that active modulation is realized by varying the voltage. Liquid crystals (LCs) have voltage dependent birefringence where the LCs are oriented with electric field lines that leads to a tuning of the refractive index as a function of applied electric field [115]. As a result, the active control is also obtained in integrated metamaterial-liquid crystal composites. Alternatively, metamaterial fabricated on semiconductors substrate allows injection and depletion of carriers of the semiconductors that actively responses to an electric bias [116]. Same operation can be done by 2D materials, for example graphene strongly modifies its plasmonic spectrum under bias or optical pumping with it covering a metamaterial [117]. However, these techniques are limited by the modulation speed. New techniques are desired for ultrafast terahertz active modulations.

Optical pumped semiconductors usually provide ultrafast carrier dynamics that have been utilized for all-optical modulation of EM waves [118-122]. Usually, laser pulses with energy larger than semiconductors band gap are incident on them to generate free carriers for speed associated with the recombination time. Among them, intra-band transition provides extremely ultrafast performance with the combination time to ~femtoseconds level [123]. Semiconductors, like germanium and GaAs, with direct band gap show picoseconds level of recombination time [124, 125]. Finally, indirect band gap of semiconductors, silicon for example, slows down the carrier recombination time to nanoseconds [118-120, 122]. All of them are significantly faster than the electric, magnetic, thermal, and mechanical actuations on active photonics and metamaterials for terahertz modulations [103]. Typically, the surface of optically pumped

semiconductors looks “metallic” for the frequencies that are below the plasma frequency ($2\pi \times 1$ THz) of the carriers for duration up to carrier recombination time. The co-incident terahertz wave on this area is highly reflected, but most importantly, the “metallization” of semiconductor surface is highly related to the optical pump intensity and wavelength. Therefore, continuous modulation is realized by simply varying optical pump power (or fluence). Moreover, it has been experimentally proved that high- Q resonances can enhanced the light-matter interaction such that the BIC states carrying infinite Q -factors are promising for low-fluence and ultrafast terahertz modulations [77, 103].

1.4 Organization of the thesis

In this thesis, diverse BIC phenomena will be realized in different dielectric metasurfaces and PhC slabs. The underlying physics of these BICs will be ambiguously revealed. The ultrafast modulation of terahertz BICs is also demonstrated. Such developments on compact terahertz meta-photonic devices will stimulate new thinking across a broad range of fields for ultimately practical applications.

Chapter 1 provides a general introduction to the background of this thesis. The brief history of terahertz technologies is reviewed. Previous efforts on photonics are introduced. Current cutting-edge progress on zero-linewidth resonance in resonant dielectric photonics and metamaterials are the main motivation of this thesis. Active control of terahertz wave is also summarized.

Chapter 2 develops the algorithm that is known as rigorous coupled-wave analysis (RCWA), also known as Fourier modal method (FMM). The RCWA algorithm, without meshing and visualizing devices, is one of the best efficient methods for simulation the diffraction coefficients of periodic metamaterials and photonics. It is employed to sweep parameters through this thesis.

Chapter 3 will introduce the first experimental demonstration of active control of high- Q supercavity resonance govern by BICs in silicon based all-dielectric terahertz metamaterials under traverse electric (TE) excitation. The low-loss, CMOS compatible, and on-chip characteristics will be shown and the high-speed (within 3 nanoseconds) and low-threshold ($10.16 \mu\text{J}/\text{cm}^2$) optical induced terahertz modulation will also be introduced.

In Chapter 4, the same device as chapter 3 under transverse magnetic (TM) polarized excitation shows guided mode resonances (GMRs) in terahertz regime. The lattice behaves simultaneously as a diffractive coupler as well as an in-plane effective slab waveguide. The non-radiative BIC state at normal incidence will also be explored. However, at oblique incidence, the in-plane wavevector allow the radiative GMRs to be guided as counter-propagating modes with identical intensities. The proposed GMR based on all-dielectric silicon metasurface could enable high- Q filters with angle-dependent spectral selectivity and free-space coupling for terahertz photonic applications.

Chapter 5 will introduce in-plane symmetry (C_{4v}) breaking of terahertz dielectric metasurface, which can excite BICs not only protected by symmetry. With in-plane symmetry breaking, additional BICs will be discussed. The physics of these new type BICs are understood as destructive interference of propagating waves at the slab-medium interface. Near the BIC state, the enhanced field localization will also be investigated as they are crucial for applications, such as low-threshold lasing (QCLs, surface emission, and VECELs, et al.), high-harmonic generation, high-sensitivity bio-/chemical sensing, and so on.

In chapter 6, a Dirac cone excited in “daisy” PhC slab will be investigated. The building blocks of low-loss material and non-radiating BIC at the Dirac cone-like dispersion enable the extremely long-distance propagation for in-plane terahertz waves. The angle-resolved

transmission spectra are measured by extremely long scan (>400 picoseconds) terahertz spectroscopy. The active control of zero-index PhC slabs will also be further discussed.

Finally, in **Chapter 7**, we provide concluding remarks and future outlooks.

Chapter 2: Rigorous coupled wave analysis for periodic gratings

2.1 Background

Initially established by M. G. Moharam and T. K. Gaylord in 1980's, the rigorous coupled-wave algorithm (RCWA), also known as Fourier modal method (FMM), is a semi-analytical Fourier space method for finding exact solutions of EM waves diffracted through intricate grating structures [126-131]. The Maxwell's equations with harmonic time dependence of $\exp(-i\omega t)$ are written as: $\nabla \cdot \epsilon_0 \epsilon_r \mathbf{E} = 0$, and $\nabla \cdot \tilde{\mathbf{H}} = 0$, $\nabla \times \tilde{\mathbf{H}} = -i\omega \epsilon_0 \epsilon_r \mathbf{E}$, and $\nabla \times \mathbf{E} = -i\omega \mu_0 \mu_r \tilde{\mathbf{H}}$, where ϵ_r is dielectric permittivity, μ_r is the dielectric permeability, and $\tilde{\mathbf{H}}$ is the actual, non-normalized field vector. The magnetic field can be normalized as $\mathbf{H} = -i\sqrt{\mu_0/\epsilon_0} \tilde{\mathbf{H}}$, and the propagating wavevector is defined as $k_0 = \omega/c = \omega\sqrt{\mu_0\epsilon_0}$. Therefore, the third and fourth equations are normalized as $\nabla \times \mathbf{H} = k_0 \epsilon_r \mathbf{E}$ and $\nabla \times \mathbf{E} = k_0 \mu_r \mathbf{H}$, where they are decomposed into three-dimensional components for Cartesian coordinates:

$$\frac{\partial E_z}{\partial y} - \frac{\partial E_y}{\partial z} = k_0 \mu_x H_x, \quad \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} = k_0 \epsilon_x E_x, \quad (2.1a)$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \mu_y H_y, \quad \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = k_0 \epsilon_y E_y, \quad (2.1b)$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0 \mu_z H_z, \quad \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} = k_0 \epsilon_z E_z. \quad (2.1c)$$

Usually, the incident EM waves are defined into TE and TM polarizations. Therefore,

TE

TM

$$-\frac{\partial E_y}{\partial z} = k_0 \mu_x H_x, \quad -\frac{\partial H_y}{\partial z} = k_0 \epsilon_x E_x, \quad (2.2a)$$

$$H_y = 0, \quad E_y = 0, \quad (2.2b)$$

$$\frac{\partial E_y}{\partial x} = k_0 \mu_z H_z, \quad \frac{\partial H_y}{\partial x} = k_0 \epsilon_z E_z, \quad (2.2c)$$

$$E_x = 0, \quad H_x = 0, \quad (2.2d)$$

$$\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} = k_0 \epsilon_y E_y, \quad \frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \mu_y H_y, \quad (2.2e)$$

$$E_z = 0, \quad H_z = 0, \quad (2.2f)$$

Substituting Eqs. (2.2a) and (2.2c) into Eq. (2.2f) and considering nonmagnetic materials, the Maxwell's equations become wave equations for electric field (E_y) for TE polarization and magnetic field (H_y) for TM polarization

$$\text{TE: } \left[\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} \right] E_y(\mathbf{r}) + k_0^2 \epsilon(\mathbf{r}) E_y(\mathbf{r}) = 0, \quad (2.3a)$$

$$\text{TM: } \frac{\partial}{\partial x} \left(\frac{1}{\epsilon(\mathbf{r})} \frac{\partial}{\partial x} H_y(\mathbf{r}) \right) + \frac{\partial}{\partial z} \left(\frac{1}{\epsilon(\mathbf{r})} \frac{\partial}{\partial z} H_y(\mathbf{r}) \right) + k_0^2 H_y(\mathbf{r}) = 0, \quad (2.3b)$$

For the RCWA algorithm, both electric field (E_y) for TE polarization, magnetic field, and the dielectric permittivity are expanded by Fourier transform such that the wave equations become eigenvalue equations. By solving these eigenvalue equations, the propagating wave vectors β are calculated as function of frequency ω or wavelength λ . By considering the boundary conditions at the interfaces of each layer, the transmission and reflection spectra can be calculated for multilayer systems. In the next few sections, different types of dielectric gratings, such as 1D binary gratings, 2D periodic gratings, and their multilayer devices, are discussed. The home developed Matlab code according to RCWA is also developed for studying BICs in this thesis.

2.2 Single layer gratings

2.2.1 Permittivity expansion for binary gratings

For simplicity, we firstly focus on single-layered grating that is uniform in y ($\partial/\partial y = 0$) and infinitely periodic in x , as shown in **Figure 2-1**. Three regions are recognized by $z = 0$ and

$z = t_g$. In region I, $z < 0$ and $\varepsilon_I = 1$, there are incoming planewave with angle θ of incidence and reflected waves. In region III, $z > t_g$ and $\varepsilon_{III} = 1$, only the transmitted waves are allowed. The region II, $0 < z < t_g$, is the grating whose solutions are modes of a periodic array of slab waveguides. The grating structure is considered as the periodically arranged dielectric ridges with permittivity of ε_g and air grooves with permittivity of ε_a .

Figure 2-1. Schematic view of single-layer binary grating.

The dielectric function $\varepsilon(x)$ is therefore expanded into Fourier series by using Fourier transform

$$\begin{aligned}
 \varepsilon_m &= \frac{1}{\Lambda_x} \int_0^{\Lambda_x} \varepsilon(x) \cos(2m\pi x / \Lambda_x) dx \\
 &= \frac{1}{\Lambda_x} \left[\int_0^{f\Lambda_x} \varepsilon_g \cos(2m\pi x / \Lambda_x) dx + \int_{f\Lambda_x}^{\Lambda_x} \varepsilon_a \cos(2m\pi x / \Lambda_x) dx \right] \\
 &= (\varepsilon_g - \varepsilon_a) \frac{\sin(m\pi f)}{m\pi}, (m \neq 0)
 \end{aligned} \tag{2.4}$$

where m is the m -th Fourier order that is an integer and truncated as $-(N-1)/2 \leq m \leq (N-1)/2$, f is the filling factor of the dielectric ridges. Here, the lateral (x, y) field components are kept tracking in the next sections. Both TE- and TM-polarized incidence are

derived for solving the (reflected and transmitted) diffractions of the grating, and the distributions of electric and magnetic fields for the device (all regions).

2.2.2 TE-polarized incidence

The electric field is oscillated along y -direction for TE-polarized incidence

$$E_{inc,y} = \exp[-ik_0(\sin\theta x + \cos\theta z)], \quad (2.5)$$

where the wavevector $k_0 = 2\pi/\lambda$ has lateral (x , in-plane) and longitudinal (z , out-of-plane) components for the angle of incidence θ .

The incident and reflected field components exist in region I, $z < 0$:

$$E_{I,y} = E_{inc,y} + \sum_m R_m \exp[-i(k_{xm}x - k_{I,zm}z)], \quad (2.6a)$$

Only transmitted electric and magnetic fields are allowed in region III, $z > t_g$:

$$E_{III,y} = \sum_m T_m \exp[-i(k_{xm}x - k_{III,zm}(z - t_g))], \quad (2.6b)$$

where $k_{xm} = k_0 \sin\theta - \frac{2m\pi}{\Lambda_x}$ denotes the lateral (in-lane) wavevector that is determined by the Floquet condition [43]. Correspondingly, the longitudinal wavevectors in regions I and III are given by $k_{\rho,zm} = \sqrt{k_0^2 - k_{xm}^2}$, where $\rho = I, III$ represents the first and third region. In Eqs. (2.6), $E_{inc,y}$ is the y -polarized incident electric field which can be reflected in region I and transmitted in region III by the grating in region III with the m -th order coefficient R_m and T_m . Each order field components are summed to obtain the total reflected and transmitted fields. This summation can be truncated by N to save calculation time if the convergence is reached. Notice that only the zeroth order of the diffraction is propagating ($k_{I,z0}$ is real) for subwavelength ($\Lambda_x < \lambda$) gratings, while the high orders are all evanescent since $k_{I,z1}$, $k_{I,z2}$, etc. are imaginary. To prevent exponentially increasing field amplitudes, the imaginary parts

of all the $k_{I,zm}$ must be negative since here the loss system is studied. The magnetic fields have two (x, z) components in these two regions can be derived from Maxwell's equations that are expressed as vectors

$$\mathbf{H}_{inc} = V_{I,0}E_{inc,y}\hat{\mathbf{x}} - K_{x0}E_{inc,y}\hat{\mathbf{z}}, \quad (2.7a)$$

$$\mathbf{H}_I = \mathbf{H}_{inc} + \sum_m [-V_{I,m}R_m \exp[-i(k_{xm}x - k_{I,zm}z)]\hat{\mathbf{x}} - K_{xm}R_m \exp[-i(k_{xm}x - k_{I,zm}z)]\hat{\mathbf{z}}], \quad (2.7b)$$

$$\mathbf{H}_{III} = \sum_m [V_{III,m}T_m \exp[-i(k_{xm}x - k_{III,zm}(z - t_g))]\hat{\mathbf{x}} - K_{xm}T_m \exp[-i(k_{xm}x - k_{III,zm}(z - t_g))]\hat{\mathbf{z}}], \quad (2.7c)$$

$$K_{xm} = \frac{ik_{xm}}{k_0}, \text{ and } V_{\rho,m} = \frac{ik_{\rho,zm}}{k_0}. \quad (2.7d)$$

where μ is the permeability (all to be 1 through this thesis) of the regions and ω is the angular frequency.

In region II, $0 < z < t_g$, the lateral electric (y -direction) and magnetic (x -direction) fields are expanded by Fourier expansion for the space-harmonic fields are

$$E_{II,y} = \sum_n S_{ym}(z) \exp(-ik_{xm}z), \quad (2.8a)$$

$$H_{II,x} = \sum_m U_{xm}(z) \exp(-ik_{xm}z), \quad (2.8b)$$

where ε_0 is the permittivity in free space [132-134]. $S_{ym}(z)$ and $U_{xm}(z)$ are the normalized amplitudes of the m -th space-harmonic fields such that $E_{II,y}$ and $H_{II,x}$ satisfy the Maxwell's equation in this region

$$\frac{\partial E_{II,y}}{\partial z} = i\omega\mu_0 H_{II,x}, \quad (2.9a)$$

$$\frac{\partial H_{II,x}}{\partial z} = -i\omega\varepsilon_0 \varepsilon(x) E_{II,y} + \frac{\partial H_{II,z}}{\partial x}, \quad (2.9b)$$

Substituting Eqs. (2.8) in to Eqs. (2.9) and eliminating $H_{II,z}$ to have

$$\frac{\partial S_{ym}}{\partial z} = k_0 U_{II,x} \quad (2.10a)$$

$$\frac{\partial U_{xm}}{\partial z} = \left(\frac{k_{xm}^2}{k_0}\right) S_{ym} - k_0 \sum_n \varepsilon_{m-n} S_{yn}, \quad (2.10b)$$

By constructing Eqs. (2.10) in matrix form [146]

$$\begin{bmatrix} \partial \mathbf{S}_y / \partial(z') \\ \partial \mathbf{U}_x / \partial(z') \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{A} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{S}_y \\ \mathbf{U}_x \end{bmatrix}, \quad (2.11)$$

which can be reduced to

$$[\partial^2 \mathbf{S}_y / \partial(z')^2] = [\mathbf{A}] [\mathbf{S}_y], \quad (2.12)$$

by defining matrix $\mathbf{A} = -\mathbf{K}_x^2 - [\varepsilon]$, where $\mathbf{K}_x$ is diagonal matrix with element of K_{xm} , $[\varepsilon]$ is the Toeplitz matrix from equation (2.4). The solutions to Eq. (2.12) compose waveguide-array modes with in-plane guided modes and out-of-plane propagating (leaky) modes that bounce back and forth by the interfaces at $z = 0$ and $z = t_g$. The forward (+z) and backward (-z) propagating components for each order have coefficients of c_m^+ and c_m^- .

$$S_{ym}(z) = \sum_n W_{m,n} \{c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)]\}, \quad (2.13a)$$

$$U_{xm}(z) = \sum_n V_{m,n} \{-c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)]\}, \quad (2.13b)$$

The field coefficients $W_{m,n}$ and $V_{m,n}$, propagating wavevectors β_n need to be solved. The eigenvalues β_n are the same as $k_{\rho,zm}$, i.e. the z -direction wavenumber, in the region (I), i.e. incidence/reflection, and region (III), i.e. transmission. There is no coupling (orthogonal) for each (m) differential equation since $\boldsymbol{\beta}$ is diagonal so the solution to equation (2.8) becomes the matrix form of equation (2.13a)

$$\mathbf{E}_y(z) = \mathbf{W} \{ \mathbf{c}^+ \exp(-k_0 \boldsymbol{\beta} z) + \mathbf{c}^- \exp[k_0 \boldsymbol{\beta} (z - t_g)] \}. \quad (2.14a)$$

or

$$E_{ym}(z) = \sum_n W_{m,n} \{c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)]\}. \quad (2.14b)$$

with $(N-1)/2 \leq n \leq (N-1)/2$. Here, $\mathbf{c}^+$ and $\mathbf{c}^-$ are constants and can be solved by the boundary conditions. Therefore, the x -component of magnetic field can now be calculated from equation (2.2b), and same for the z -component from (2.2f). By defining $\mathbf{V} = \mathbf{W}\boldsymbol{\beta}$ we have

$$\mathbf{H}_x(z) = \mathbf{V} \{-\mathbf{c}^+ \exp(-k_0 \boldsymbol{\beta} z) + \mathbf{c}^- \exp[k_0 \boldsymbol{\beta} (z - t_g)]\}. \quad (2.15a)$$

or

$$H_{xm}(z) = \sum_n V_{m,n} \{-c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)]\}. \quad (2.15b)$$

We also define the diagonal matrices $\boldsymbol{\Phi}(z) = \exp(-k_0 \boldsymbol{\beta} z)$ and $\mathbf{X} = \boldsymbol{\Phi}(t_g)$. Equations (2.14) and (2.15) are now written in a concise form as

$$\begin{bmatrix} \mathbf{E}_y(z) \\ \mathbf{H}_x(z) \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ \mathbf{V} & -\mathbf{V} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Phi}(z) & \mathbf{0} \\ \mathbf{0} & \mathbf{X}\boldsymbol{\Phi}(-z) \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}. \quad (2.16)$$

The individual field harmonics (intensity) are expressed by the n -th column of the eigenvector matrices $\mathbf{W}$ and $\mathbf{V}$, i.e. $\mathbf{W}_n$ and $\mathbf{V}_n \mathbf{B}$, that compose the eigenmodes of the grating structure. $\mathbf{W}_n$ and $\mathbf{V}_n$ are the standard electric and magnetic basis vectors of the structure. Similarly, the electric and magnetic fields in the homogeneous regions I and III can be expressed in the same way as

$$\begin{bmatrix} \mathbf{E}_{I,y}(z) \\ \mathbf{H}_{I,x}(z) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_I & \mathbf{W}_I \\ \mathbf{V}_I & -\mathbf{V}_I \end{bmatrix} \begin{bmatrix} \boldsymbol{\Phi}_I(z) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Phi}_I(-z) \end{bmatrix} \begin{bmatrix} \delta_0 \\ \mathbf{R} \end{bmatrix}, \quad (2.17a)$$

$$\begin{bmatrix} \mathbf{E}_{III,y}(z) \\ \mathbf{H}_{III,x}(z) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_{III} & \mathbf{W}_{III} \\ \mathbf{V}_{III} & -\mathbf{V}_{III} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Phi}_{III}(z - t_g) & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Phi}_{III}(t_g - z) \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{0} \end{bmatrix}. \quad (2.17b)$$

Eqs. (2.16) and (2.17) have four unknown matrices $\mathbf{R}$, $\mathbf{T}$, $\mathbf{c}^+$, and $\mathbf{c}^-$. To solve them, the boundary conditions of the EM fields can be applied at $z = 0$ and $z = t_g$, which read

$$\begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{V}_I & -\mathbf{V}_I \end{bmatrix} \begin{bmatrix} \delta_0 \\ \mathbf{R} \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W}\mathbf{X} \\ \mathbf{V} & -\mathbf{V}\mathbf{X} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}, \quad (2.18a)$$

$$\begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{V}_{III} & -\mathbf{V}_{III} \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{W}\mathbf{X} & \mathbf{W} \\ \mathbf{V}\mathbf{X} & -\mathbf{V} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}. \quad (2.18b)$$

Here $\mathbf{R}$ can be eliminated from (2.18a) and $\mathbf{T}$ can be eliminated from (2.18b), and two equations are concatenated in a single matrix equation

$$\begin{bmatrix} 2\mathbf{V}_I\delta_0 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{W}\mathbf{V}_I + \mathbf{V} & (\mathbf{W}\mathbf{V}_I - \mathbf{V})\mathbf{X} \\ (\mathbf{W}\mathbf{V}_{III} - \mathbf{V})\mathbf{X} & \mathbf{W}\mathbf{V}_{III} + \mathbf{V} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}. \quad (2.19)$$

Eq. (2.19) is employed to solve $\mathbf{c} = [\mathbf{c}^+ \quad \mathbf{c}^-]^T$ where T stands for transpose. Substituting $\mathbf{c}$ into (2.18), $\mathbf{R}$ and $\mathbf{T}$ are obtained as

$$\begin{bmatrix} \mathbf{I} \\ -\mathbf{V}_I \end{bmatrix} \mathbf{R} = \begin{bmatrix} \mathbf{W} & \mathbf{W}\mathbf{X} \\ \mathbf{V} & -\mathbf{V}\mathbf{X} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix} - \begin{bmatrix} \mathbf{I} \\ -\mathbf{V}_I \end{bmatrix} \delta_0, \quad (2.20a)$$

$$\begin{bmatrix} \mathbf{I} \\ \mathbf{V}_{III} \end{bmatrix} \mathbf{T} = \begin{bmatrix} \mathbf{W} & \mathbf{W}\mathbf{X} \\ \mathbf{V} & -\mathbf{V}\mathbf{X} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}. \quad (2.20b)$$

Finally, the m -th order efficiencies of diffraction for the reflection and transmission, i.e. RD_m and TD_m , are calculated as

$$RD_m = |R_m|^2 \operatorname{Re} \left(\frac{\gamma_{I,m}}{\gamma_{I,0}} \right), \quad (2.21a)$$

$$TD_m = |T_m|^2 \operatorname{Re} \left(\frac{\gamma_{III,m}}{\gamma_{III,0}} \right). \quad (2.21b)$$

where $\operatorname{Re}(x)$ denotes the real parts of x .

The last step is to find the field amplitudes in each region. In fact, the transverse field components have been expressed in Eq. (2.15). By combining the longitudinal component $\mathbf{H}_z$, we have

$$\begin{bmatrix} \mathbf{E}_y(z) \\ \mathbf{H}_x(z) \\ \mathbf{H}_z(z) \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ \mathbf{V} & -\mathbf{V} \\ -\mathbf{V}_z & -\mathbf{V}_z \end{bmatrix} \begin{bmatrix} \Phi_I(z) & \mathbf{0} \\ \mathbf{0} & \Phi_I(-z) \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}. \quad (2.22)$$

From equation (2.1c) where $E_x = 0$, $k_0 H_x = \partial_y E_y$, we obtain $\mathbf{H}_z = -\mathbf{K}_x \mathbf{E}_y$, which implies that

$$\mathbf{V}_z = \mathbf{K}_x \mathbf{W}. \quad (2.23)$$

The same equation has been described for the z-propagating fields in all three regions such that this result can be generalized. In Eq. (2.22), the eigenmatrices $[\mathbf{W} \quad \mathbf{V} \quad \mathbf{V}_z]$ is expressed as $\mathbf{M}$, where the coupling information is involved. On the left side of Eq. (2.22), we write the middle matrix as $\Phi(z)$. Therefore, we have

$$\Psi_I(z) = \mathbf{M}_I \Phi_I(z) \mathbf{c}_I, \quad (2.24a)$$

$$\Psi_{III}(z) = \mathbf{M}_{III} \Phi_{III}(z) \mathbf{c}_{III}, \quad (2.24a)$$

where all non-zero field components in each region is written in matrix $\Psi_{I/III} = [\mathbf{E}_y(z) \quad \mathbf{H}_x(z) \quad \mathbf{H}_z(z)]^T$. Multiplied each of these components with $\Phi_x(x) = \exp(-k_0 \mathbf{K}_x x)$, the complex magnitude at any point in the (x, z) plane of that field component is calculated. Therefore, define Φ_x as

$$\Phi_x(x) = \begin{bmatrix} \Phi_x(x) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \Phi_x(x) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \Phi_x(x) \end{bmatrix}, \quad (2.25)$$

The fields diffracted by the single layer gratings are expressed as

$$\Phi_I(x, z) = \Phi_x(x) \mathbf{M}_I \Phi_I(z) \mathbf{c}_I, \quad (2.26a)$$

$$\Phi_{III}(x, z) = \Phi_x(x) \mathbf{M}_{III} \Phi_{III}(z) \mathbf{c}_{III}, \quad (2.26b)$$

To verify the algorithm, we calculate a single-layer grating for observing BICs in Ref. [97].

The 1D binary grating composes of simple array of air grooves in silicon membrane with periodicity of Λ and refractive index $n_g = 3.5$ embedded in air, as shown in **Figure 2-2(a)**.

Figure 2-2(b) shows the transmission intensity $T(\lambda, t_g) = |t_{TE}(\lambda, t_g)|^2$ as functions of the wavelength λ and the slab thickness t_g , both normalized to the grating period Λ , for an incident angle of $\theta = 10^\circ$. Several particular features, for example $(\lambda/\Lambda, t_g/\Lambda) = (1.992, 0.702)$ and $(\lambda/\Lambda, t_g/\Lambda) = (2.065, 1.05)$, are observed as the transmission map with the signature of Fano resonances [84]. A rapid variation from near-unity to near-zero that is known as Fano resonance. The arrows shown in **Figure 2-2(b)** correspond to the resonant excitation of a leaky mode supported by the 1D grating slab [84]. These points correspond to the BICs, and the numbers of BICs are more and more as increasing the thickness of the grating.

Figure 2-2. Study single-layer binary grating with TE-polarized RCWA algorithm. (a) Dielectric lamellar 1D grating and (b) transmission map as function of the wavelength and

grating thickness (both normalized to the grating period). The black arrows indicate transmission singularities where both wavelength and thickness are confirmed for observing BICs [84].

2.2.3 TM-polarized incidence

Interaction between the TM-polarized wave and 1D grating follows the same process as the TE-polarized incidence. The convergence is time consuming as it needs much more harmonics. Same grating in **Figure 2-1** is employed here.

The incident magnetic field is unchanged along y-axis:

$$H_{inc,y} = \exp[-ik_0(\sin\theta x + \cos\theta z)], \quad (2.27)$$

The field components in region I ($z < 0$) and region III ($z > t_g$)

$$H_{I,y} = H_{inc,y} + \sum_m R_m \exp[-i(k_{xm}x - k_{I,zm}z)], \quad (2.28a)$$

$$H_{III,y} = \sum_m T_m \exp[-i(k_{xm}x - k_{III,zm}(z - t_g))], \quad (2.28b)$$

The normalized m -th order transmission and reflection coefficient R_m and T_m . k_{xm} , $k_{I,zm}$ and $k_{III,zm}$ are defined in previous section. The electric-field vectors in two regions are obtained from derivation of the Maxwell's equation. In the grating region II, $0 < z < t_g$, the lateral magnetic and electric field components in x - y -directions can be expanded in Fourier space [135]

$$H_{II,y} = \sum_m U_{ym}(z) \exp(-ik_{xm}x), \quad (2.29a)$$

$$E_{II,x} = \sum_m S_{xm}(z) \exp(-ik_{xm}x), \quad (2.29b)$$

U_{ym} and S_{xm} are normalized field amplitudes for the m -th order space harmonics such that $H_{II,y}$ and $E_{II,x}$ satisfy the Maxwell's equation

$$\frac{\partial H_{II,y}}{\partial z} = -i\omega\varepsilon_0\varepsilon(x)E_{II,x}, \quad (2.30a)$$

$$\frac{\partial E_{II,x}}{\partial z} = -i\omega\mu_0 H_{II,y} + \frac{\partial E_{II,x}}{\partial x}, \quad (2.30b)$$

To obtain the coupled-wave equations in matrix form, Eqs. (2.29a) and (2.29b) are substituting into Eqs. (2.30a) and (2.30b), respectively, and eliminating $H_{II,z}$

$$\begin{bmatrix} \partial \mathbf{U}_y / \partial(z') \\ \partial \mathbf{S}_x / \partial(z') \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \llbracket \varepsilon \rrbracket \\ \mathbf{B} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{U}_y \\ \mathbf{S}_x \end{bmatrix}, \quad (2.31)$$

which can be reduced to

$$[\partial^2 \mathbf{U}_y / \partial(z')^2] = [\llbracket \varepsilon \rrbracket \mathbf{B}] [\mathbf{U}_y], \quad (2.32)$$

where $\mathbf{B} = \mathbf{K}_x \llbracket \varepsilon \rrbracket^{-1} \mathbf{K}_x - \mathbf{I}$ with $\llbracket \varepsilon \rrbracket$ and $\mathbf{K}_x$ defined in Eq. (2.7). Same as the TE polarization incidence, coupled-wave equations are solved by calculating the eigenvalue and the eigenvectors associated with the matrix $\llbracket \varepsilon \rrbracket \mathbf{B}$. The field components contain the forward (+z) and backward (-z) propagating components for each order have coefficients of c_m^+ and c_m^- , where their space harmonics are

$$U_{ym}(z) = \sum_n W_{m,n} \{ c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)] \}, \quad (2.33a)$$

$$S_{xm}(z) = \sum_n V_{m,n} \{ -c_n^+ \exp(-k_0 \beta_n z) + c_n^- \exp[k_0 \beta_n (z - t_g)] \}, \quad (2.33b)$$

Here in Eqs. (2.33) $W_{m,n}$ are the elements of the eigenvector matrix $\mathbf{W}$, β_n are the positive square root of the eigenvalues of the matrix $\llbracket \varepsilon \rrbracket \mathbf{B}$, and $V_{m,n}$ are the matrix elements of $\mathbf{V} = \llbracket \varepsilon \rrbracket^{-1} \mathbf{W} \mathbf{\Gamma}$ with $\mathbf{\Gamma}$ being a diagonal matrix with the diagonal elements β_n . Therefore, the

amplitudes of the diffracted fields R_m and T_m together with propagating coefficients of c_m^+ and c_m^- are determined from the boundary condition. By matching the lateral field at the input ($z = 0$) and output ($z = t_g$) boundaries, we have

$$\delta_{m0} + R_m = \sum_n W_{m,n} \{c_n^+ + c_n^- \exp(-k_0 \beta_n t_g)\}, \quad (2.34a)$$

$$i \left[\cos \theta \delta_{m0} - \frac{k_{I,zm}}{k_0} R_m \right] = \sum_n V_{m,n} \{c_n^+ - c_n^- \exp(-k_0 \beta_n t_g)\}, \quad (2.34a)$$

$$\sum_n V_{m,n} \{c_n^+ \exp(-k_0 \beta_n t_g) + c_n^-\} = T_m, \quad (2.34c)$$

$$\sum_n V_{m,n} \{c_n^+ \exp(-k_0 \beta_n t_g) + c_n^-\} = K_{I,zm} T_m, \quad (2.34d)$$

which can be written in matrix form as

$$\begin{bmatrix} \delta_{m0} \\ i \delta_{m0} \cos \theta \end{bmatrix} + \begin{bmatrix} \mathbf{I} \\ -\mathbf{Z}_I \end{bmatrix} [\mathbf{R}] = \begin{bmatrix} \mathbf{W} & \mathbf{WX} \\ \mathbf{V} & -\mathbf{VX} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix}, \quad (2.35a)$$

$$\begin{bmatrix} \mathbf{W} & \mathbf{WX} \\ \mathbf{V} & -\mathbf{VX} \end{bmatrix} \begin{bmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{bmatrix} = \begin{bmatrix} \mathbf{I} \\ i \mathbf{Z}_{III} \end{bmatrix} [\mathbf{T}], \quad (2.35b)$$

These two equations are solved simultaneously for the reflected and transmitted amplitudes of diffracted fields. Same to the TE-polarized case, the propagating coefficients c_m^+ and c_m^- are expressed and then substituting them back to Eqs. (2.34c) and (2.34d) to find the diffraction efficiencies as

$$RD_m = |R_m|^2 \operatorname{Re} \left(\frac{k_{I,zm}}{k_0 \cos \theta} \right), \quad (2.36a)$$

$$TD_m = |T_m|^2 \operatorname{Re} \left(\frac{k_{I,zm}}{k_0 \cos \theta} \right). \quad (2.36b)$$

Figure 2-3. Excitation of BIC in 1D binary grating with TM-polarized plane wave. (a) Transmission map as function of the wavelength and grating thickness (both normalized to the grating period) under angle of incidence $\theta = 10^\circ$. The black arrows indicate two transmission singularities, with coordinates $(\lambda/\Lambda, t_g/\Lambda) = (2.042, 0.973)$ and $(\lambda/\Lambda, t_g/\Lambda) = (2.524, 1.31)$, where both wavelength and thickness are confirmed for observing BICs. (b) Transmission map as function of the incident angle and the wavelength with normalized geometric thickness $t_g/\Lambda = 1.31$. The BIC is recognized at $(\lambda/\Lambda, t_g/\Lambda) = (2.524, 10)$. Both (a) and (b) are excited by the TM-polarized excitation.

2.3 Multilayer binary gratings

The single-layer binary grating has been studied for calculating the EM field diffractions. Now, the algorithm needs to be extended to multilayer structures. In this case, the grating is also periodic modulation of permittivity $\varepsilon(x) = \varepsilon(x + m\Lambda_x)$ in x -direction and uniform ($\partial/\partial y = 0$) in y -direction. However, the dielectric function may change along the wave propagating (z -axis) direction as $\varepsilon(z + m\Lambda_z, z)$. The straight solutions for Maxwell's equation for such systems are not practical by employing the entire to be single layer. The feasible solutions to them can be broken to form multilayers in z -direction, and each layer is expressed by Fourier

expansions. Boundary conditions for each interface of different layers are matched and compacted into a transfer (T-) matrix or scattering (S-) matrix. Therefore, the multilayer binary system is numerically solved [136-141]. In practice, the T-matrix is numerically badly behaved for patterned multilayers since they have in-plane wavevectors $(k_0 \sin \theta - \frac{2m\pi}{\Lambda_x})$. These in-plane wavevectors exhibit strongly evanescent behaviors in z-direction that rapidly leads to numerical overflow. We therefore only employ the S-matrix for dealing with patterned multilayer gratings. First, the structure is approximated in such a way that the theory developed in the previous sections can still work. Here, two functions are defined as the l -th layer filling factor $f(z) = f_l$ and the l -th layer thickness $h(z) = h_l$. Particularly, L is the total number of layers, among which the superstrate is the first layer ($l = 0$) and the substrate layer is the last layer ($l = L$) such that the filling factor $f_0 = f_L$ is unit. The field components in the superstrate and substrate are therefore same as the fields in regions I and III for the single-layer grating. However, the left $L-2$ layers need to be expanded by Fourier transform. The permittivity for each layer has form of $\llbracket \varepsilon_l \rrbracket$, where the eigenequations for both TE- and TM-polarizations are given by Eqs. (2.16) and (2.36), respectively. Finally, boundary conditions at each interface are applied. Combining with S-matrix method, the m -th order reflection R_m and transmission T_m coefficients can be obtained. Here, the stepwise algorithm is demonstrated.

The S-matrix is schematically shown in **Figure 2-4(a)**, where the system contains two input ports and two output ports. A linear relation between the inputs and outputs is defined for the S-matrix of this system. In quantum mechanics, an operator is used such that it applies to the incoming wavefunction for computing the outgoing waves, $\psi_{out} = \hat{S}\psi_{in}$. For the system we study

$$\begin{bmatrix} T \\ R \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} I^+ \\ I^- \end{bmatrix}, \quad (2.37)$$

from which we have

$$T = S_{11}I^+ + S_{12}I^-, \quad (2.38a)$$

$$R = S_{21}I^+ + S_{22}I^-, \quad (2.38b)$$

Now the device is connected by two systems $S^{(1)}$ and $S^{(2)}$. The forward propagating c^+ outgoing from $S^{(1)}$ acts as the input of $S^{(2)}$. On the contrary, the backward propagating c^- from $S^{(2)}$ is the input of $S^{(1)}$. Here, c^+ and c^- are unknown but they can be eliminated by applying linear algebra as [137-141]

$$S_{11} = S_{11}^{(2)} \left(I - S_{12}^{(1)} S_{21}^{(2)} \right)^{-1} S_{11}^{(1)}, \quad (2.39a)$$

$$S_{12} = S_{12}^{(2)} + S_{11}^{(2)} S_{12}^{(1)} \left(I - S_{21}^{(2)} S_{12}^{(1)} \right)^{-1} S_{22}^{(2)}, \quad (2.39b)$$

$$S_{21} = S_{21}^{(1)} + S_{22}^{(1)} S_{21}^{(2)} \left(I - S_{12}^{(1)} S_{21}^{(2)} \right)^{-1} S_{11}^{(1)}, \quad (2.39c)$$

$$S_{22} = S_{22}^{(1)} \left(I - S_{21}^{(2)} S_{12}^{(1)} \right)^{-1} S_{22}^{(2)}, \quad (2.39d)$$

This relationship is usually denoted $S = S^{(1)} \otimes S^{(2)}$. Now the system contains L layers. For any l -th interface

$$S^l = \begin{bmatrix} W_{l+1} & -W_l \\ V_{l+1} & V_l \end{bmatrix}^{-1} \begin{bmatrix} W_l X_l & -W_{l+1} X_{l+1} \\ V_l X_l & V_{l+1} X_{l+1} \end{bmatrix}. \quad (2.40)$$

The overall S-matrix is finally written as $S = S^{(1)} \otimes S^{(2)} \otimes \dots \otimes S^{(L-1)}$ since the L^{th} layer is the substrate. Once S-matrix fixed, the wave amplitudes for diffractions (i.e. transmission and reflection) are computed from Eq. (2.37). For a monochromatic wave with unit-amplitude that is single direction incidence, we have

$$T = S_{11}\delta_0, \text{ and } R = S_{21}\delta_0. \quad (2.41)$$

Figure 2-4. Discovery Dirac-cone dispersion in multilayered 1D gratings [142]. (a) The S-matrix for single layer (up) and bi-layer (down) devices, respectively. (b) The band structures of TE (red) and TM (blue) polarizations calculated by COMSOL. The inset figure is the unit cell of the multilayer silicon ($\epsilon = 11.7$) grating, where the period $\Lambda = 600 \text{ nm}$, the width and height of grating are $w = t = 0.35\Lambda$. (c) and (d) The magnetic and electric fields at Γ point for TE (TE₁, TE₂ and TE₃) and TM (TM₁, TM₂ and TM₃) bands, respectively. (e) and (f) The

angle-resolved transmission spectra as function of incident angle (θ) and frequency (in terahertz) calculated by using RCWA algorithm. (e) TE polarization and (f) TM polarization, from where the ten layers of silicon gratings were taken into calculations. All the polarizations were defined according to ref. [142].

The S-matrix implementation was verified by using a multilayer photonic structure that excites Dirac-cone under TM-polarized excitation, as shown in **Figure 2-4**. **Figure 2-4(a)** shows the derivation of the S-matrix from single-layer device, given by Eqs. (2.38), and the bi-layer device, given by Eqs. (2.39). The band structures for TE-/TM-polarization were calculated by COMSOL eigenmode analysis with the FEM method, as shown in **Figures 2-4(b)**. The TE-polarized bands are plotted in red dots and the TM-polarized band is shown in blue one. The mode profiles for TE-/TM-polarizations are shown in **Figures 2-4(c)** and **2-4(d)**, where the terminology of TE or TM bands stems from electric field (H_z , TE-polarization) and magnetic field (E_z , TM-polarization) [142]. It is clearly shown that the multilayer photonics support a Dirac cone dispersion in both band structures and angle-resolved transmission under TM-polarized far-field excitation, as shown in **Figures 2-4(b)** and **2-4(f)**. The angle-resolved transmission spectra for the TE-polarized incidence are also demonstrated in **Figure 2-4(e)**, from which we can verify the vitality of the RCWA algorithm. Later, this Dirac-cone dispersion will be employed for low-loss zero-index BICs in **Chapter 6**.

Finally, the field profiles for given wavelength (frequency) need to be visualized, while S-matrix eliminates the amplitude coefficients of the internal layers and T-matrix is numerically unstable due to the evanescent behavior for the in-plane wavevectors [138-141]. The feasible solution to this could be putting the amplitude coefficients of all layers and outgoing waves R and T inside a column matrix $\mathcal{C}$. Same operation is applied to the field amplitudes where this column matrix is defined as $\mathcal{F}$.

$$\mathcal{C} = \begin{bmatrix} \mathbf{I}^+ \\ \mathbf{R} \\ \mathbf{c}_2^+ \\ \mathbf{c}_2^- \\ \mathbf{c}_3^+ \\ \vdots \\ \mathbf{c}_{L-1}^+ \\ \mathbf{c}_{L-1}^- \\ \mathbf{T} \\ \mathbf{I}^- \\ \mathbf{R} \\ \mathbf{T} \end{bmatrix}, \text{ and } \mathcal{F} = \begin{bmatrix} \mathbf{E}_{inc} \\ \mathbf{H}_{inc} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}. \quad (2.42)$$

where the entire matrix $\mathcal{C}$ is unknown in most cases even though $\mathbf{I}^+ = \delta_0$ and $\mathbf{I}^- = 0$ (single-direction incidence). To find the incident fields, a big matrix $\mathcal{B}$ is defined as

$$\mathcal{B}\mathcal{C} = \mathcal{F}, \text{ or } \mathcal{C} = \mathcal{B}^{-1}\mathcal{F}. \quad (2.43)$$

First, we test the big matrix $\mathcal{B}$ for the single-layer binary grating. At every interface, the fields are expressed by using the coefficients in $\mathcal{C}$. For the first interface ($z = 0^-$), the incident and reflected fields are defined

$$\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ \mathbf{V}_1 & -\mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{I}^+ \\ \mathbf{R} \end{bmatrix} - \begin{bmatrix} \mathbf{W}_1 \\ -\mathbf{V}_1 \end{bmatrix} \mathbf{R} = \begin{bmatrix} \mathbf{E}_{inc} \\ \mathbf{H}_{inc} \end{bmatrix}. \quad (2.44a)$$

For the same interface ($z = 0^+$) from the grating layer

$$-\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ \mathbf{V}_1 & -\mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{I}^+ \\ \mathbf{R} \end{bmatrix} + \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2\mathbf{X} \\ \mathbf{V}_2 & -\mathbf{V}_2\mathbf{X} \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix} = \begin{bmatrix} \mathbf{E}_{inc} \\ \mathbf{H}_{inc} \end{bmatrix} \quad (2.44b)$$

Same operation is applied to the outgoing interface

$$-\begin{bmatrix} \mathbf{W}_2\mathbf{X} & \mathbf{W}_2 \\ \mathbf{V}_2\mathbf{X} & -\mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{bmatrix} + \begin{bmatrix} \mathbf{W}_3 & \mathbf{W}_3 \\ \mathbf{V}_3 & -\mathbf{V}_3 \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}. \quad (2.44c)$$

$$-\begin{bmatrix} \mathbf{W}_3 & \mathbf{W}_3 \\ \mathbf{V}_3 & -\mathbf{V}_3 \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{W}_3 \\ \mathbf{V}_3 \end{bmatrix} \mathbf{T} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}. \quad (2.44d)$$

The column matrices defined before become $\mathcal{C} = [\delta_0 \quad \mathbf{R} \quad \mathbf{c}_2^+ \quad \mathbf{c}_2^- \quad \mathbf{T} \quad \mathbf{0} \quad \mathbf{R} \quad \mathbf{T}]$, and $\mathcal{F} = [\mathbf{E}_{inc} \quad \mathbf{H}_{inc} \quad \mathbf{0} \quad \mathbf{0} \quad \mathbf{0} \quad \mathbf{0} \quad \mathbf{0} \quad \mathbf{0}]$. As results, the big matrix is constructed as

$$\mathcal{B} = \begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{W}_1 & \mathbf{0} \\ \mathbf{V}_1 & -\mathbf{V}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{V}_1 & \mathbf{0} \\ -\mathbf{W}_1 & -\mathbf{W}_1 & \mathbf{W}_2 & \mathbf{W}_2 \mathbf{X}_2 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ -\mathbf{V}_1 & \mathbf{V}_1 & \mathbf{V}_2 & -\mathbf{V}_2 \mathbf{X}_2 & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{W}_2 \mathbf{X}_2 & -\mathbf{W}_2 & \mathbf{W}_3 & \mathbf{W}_3 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{V}_2 \mathbf{X}_2 & \mathbf{V}_2 & \mathbf{V}_3 & -\mathbf{V}_3 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{W}_3 & -\mathbf{W}_3 & \mathbf{0} & \mathbf{W}_3 \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & -\mathbf{V}_3 & \mathbf{V}_3 & \mathbf{0} & \mathbf{V}_3 \end{bmatrix}. \quad (2.45)$$

which satisfies Eq. (2.43). Here, the Eq. (2.45) is an expression from the four parts of Eqs. (2.44) in a single matrix. From this $\mathcal{B}$ matrix, one could extend it into multilayer. First, we define the sub-matrix with lowercase $\mathbf{b}_\rho$ with ρ as layer number. Therefore,

$$\mathbf{b}_\rho = \begin{bmatrix} \mathbf{W}_\rho & \mathbf{W}_\rho \mathbf{X}_\rho \\ \mathbf{V}_\rho & -\mathbf{V}_\rho \mathbf{X}_\rho \\ -\mathbf{W}_\rho \mathbf{X}_\rho & -\mathbf{W}_\rho \\ -\mathbf{V}_\rho \mathbf{X}_\rho & \mathbf{V}_\rho \end{bmatrix}. \quad (2.46)$$

By arranging the sub-matrices $\mathbf{b}$ inside $\mathcal{B}$, the eigenvector matrices of the last two columns are added for the reflected and transmitted waves. The approach that was presented in section 2.2.2 is employed to calculate the fields. Multilayer is considered in the grating such that for Eq. 2.46, we have $\rho = 1, 2, \dots, L$. Therefore, $\Phi_\rho(z)$ must be slightly modified. In addition, $\mathcal{C}_\rho$ contains the amplitude coefficients of the forward and backward propagations for the ρ -th layer at the incoming and outgoing interface, respectively. Therefore, by subtracting the z -coordinate at the start of that layer, we correct the z -coordinate for each layer. Therefore, it becomes

$$\Phi_\rho(z) = \begin{bmatrix} \Phi_\rho(z - z_\rho) & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_\rho \Phi_\rho(z - z_\rho) \end{bmatrix}, z_{\rho-1} < z < z_\rho. \quad (2.47)$$

The rest of the process for calculating the fields is the same as section 2.2.3. The first step is to figure out the layer, for any point (x, z) , to find which it belongs. After all, by using Eq. (2.26), all the fields can be computed for that layer

$$\Phi_\rho(x, z) = \Phi_x(x) \mathbf{M}_\rho \Phi_\rho(z) \mathbf{C}_\rho. \quad (2.48)$$

Figure 2-5. Field profile of the multilayer gratings for TE-/TM-polarizations.

To calculate the field distributions for TE and TM polarization, the grating is set as 5 periods in x -axis and 10 periods in z -axis. The plane wave was employed to excite the grating at $z = -3104.5$ nm. The frequency for TM-polarization was set at the Dirac cone, while it is TE_2 band at Γ point for the TE-polarization. For TE-polarization, the real parts of the magnetic field (H_z) is plotted, as shown in **Figure 2-5(a)**. For TE-polarization, the real parts of the electric field

(E_z) is plotted, as shown in **Figure 2-5(b)**. Both polarizations show similar field profiles as the eigenmode analysis in **Figure 2-4**.

2.4 2D gratings

In this section, the algorithm is further extended to 2D case, where the device is periodic in both x - and y -directions (even in z -direction). Therefore, the permittivity (ϵ) and permeability (μ) can vary across 2D space. Any kind of photonic lattice can be analyzed using this algorithm as long as the lattice can be simplified as periodic in x - and y -directions. Only single-layer structure is solved in this section, but the multilayer solutions follow the same process as we discussed in previous section. Noponen and Turunen developed the seminal theoretical framework in 1994 [143], and three years later, it was improved by Li in 1997 [144]. Here, we follow their theoretical frame. The device composes of cubical building blocks with widths of w_x and w_y in a rectangular (or square) lattice with periods of Λ_x and Λ_y , as shown in **Figure 2-6**. The height of the grating is t_g . The dielectric permittivity of the building blocks is ϵ_g , and the surrounding medium is free space (air) with permittivity of ϵ_a .

Figure 2-6. Schematic representation of a 2D grating that has periodic boundary condition along x -/ y -axis and truncated (finite thickness) interfaces along z -axis.

The electric fields in the homogenous regions are expressed as

$$E_R(\mathbf{r}) = \sum_{m,n} R_{mn} \exp(i\mathbf{k}_{I,mn} \cdot \mathbf{r}), \quad (2.49a)$$

$$E_T(\mathbf{r}) = \sum_{m,n} T_{mn} \exp(i\mathbf{k}_{III,mn} \cdot \mathbf{r}), \quad (2.49b)$$

where $m = \pm 1, \pm 2, \dots, \pm m_{max}$, and $n = \pm 1, \pm 2, \dots, \pm n_{max}$ that denote the truncation (space harmonics) numbers along x - and y -directions. The wavevector $\mathbf{k}_{\rho,mn} = k_{xmn}\hat{x} + k_{ymn}\hat{y} + k_{\rho,zmn}\hat{z}$ with

$$k_{xmn} = k_0 \sin\theta \cos\phi + G_x, \quad (2.50a)$$

$$k_{ymn} = k_0 \sin\theta \sin\phi + G_y, \quad (2.50b)$$

where we define $G_x = 2m\pi/\Lambda_x$, $G_y = 2n\pi/\Lambda_y$, and $\mathbf{G} = G_x\hat{x} + G_y\hat{y}$. Therefore,

$$k_{\rho,zmn} = [k_0^2 - k_{xmn}^2 - k_{ymn}^2]^{1/2}. \quad (2.50c)$$

The magnetic fields are therefore obtained by calculating $\mathbf{H} = \left(\frac{i}{\omega\mu}\right) \nabla \times \mathbf{E}$,

$$\mathbf{H}_R(\mathbf{r}) = \frac{i}{k_0} \sum_{m,n} \mathbf{k}_{I,mn} \times \mathbf{R}_{mn} \exp(i\mathbf{k}_{I,mn} \cdot \mathbf{r}), \quad (2.51a)$$

$$\mathbf{H}_T(\mathbf{r}) = \sum_{m,n} \mathbf{k}_{III,mn} \times \mathbf{T}_{mn} \exp(i\mathbf{k}_{III,mn} \cdot \mathbf{r}), \quad (2.51b)$$

We calculate the z -component field amplitude from the x - and y -components in coefficient column matrix $\mathbf{C} = [C_x \ C_y]^T$ by the orthogonality of the modes. The field matrices $\mathbf{E}$ and $\mathbf{H}$ is given by a similar treatment. Therefore, the magnetic field in region ρ can be expressed as

$$\mathbf{H}_\rho = \mathbf{V}_\rho \mathbf{E}_\rho, \quad (2.52)$$

where $\mathbf{V} = \begin{bmatrix} V_{xx} & V_{xy} \\ V_{yx} & V_{yy} \end{bmatrix}$. The elements of the constituent diagonal matrices are written as

$$V_{xxj} = i \frac{k_{xj}k_{yj}}{k_0k_{zp}}, V_{xyj} = i \frac{k_{yj}+k_{zj}^2}{k_0k_{zp}}, V_{yxj} = i \frac{k_{xj}+k_{zj}^2}{k_0k_{zp}}, V_{yyj} = -V_{xxj}. \quad (2.53)$$

The diagonal matrix $\mathbf{K}_y$ with elements $K_{yn} = ik_{yn}/k_0$ is also defined. It is the same the definition for $\mathbf{K}_x$ in Eq. (2.7d).

To solve the eigenmodes in the grating region, the Fourier expansion of the permittivity has to be transformed in both directions [145, 146]

$$\varepsilon_{mn} = \frac{1}{\Lambda_x \Lambda_y} \int_0^{\Lambda_x} \int_0^{\Lambda_y} \varepsilon(x, y) \exp[-i(G_x x + G_y y)] dx dy, \quad (2.54)$$

For different geometric shapes on certain lattice structures, Eq. (2.54) exist analytical form. Here we list some of them.

For the cubical building blocks on a rectangular lattice,

$$\varepsilon_{\mathbf{G}\mathbf{G}'} = \varepsilon_g \delta_{\mathbf{G}\mathbf{G}'} + (\varepsilon_g - \varepsilon_a) \frac{\sin[(G_x - G'_x)W_x/2]}{(G_x - G'_x)\Lambda_x/2} \frac{\sin[(G_y - G'_y)W_y/2]}{(G_y - G'_y)\Lambda_y/2}. \quad (2.55)$$

For a cylinder building blocks (with radius of r) on rectangular lattice

$$\varepsilon_{\mathbf{G}\mathbf{G}'} = \begin{cases} \varepsilon_a + (\varepsilon_g - \varepsilon_a) \frac{\pi r^2}{\Lambda_x \Lambda_y}, & \mathbf{G} = \mathbf{G}' \\ 2(\varepsilon_g - \varepsilon_a) \frac{J_1(|\mathbf{G} - \mathbf{G}'|r)}{|\mathbf{G} - \mathbf{G}'|r} \frac{\pi r^2}{\Lambda_x \Lambda_y}, & \mathbf{G} \neq \mathbf{G}' \end{cases}. \quad (2.56)$$

For cylinder building blocks (with radius of r) on a hexagonal lattice ($\Lambda_x = \Lambda$, $\Lambda_y = \sqrt{3}\Lambda$)

$$\varepsilon_{\mathbf{G}\mathbf{G}'} = \begin{cases} \varepsilon_a + (\varepsilon_g - \varepsilon_a) \frac{2\pi r^2}{\sqrt{3}\Lambda^2}, & \mathbf{G} = \mathbf{G}' \\ 2(\varepsilon_g - \varepsilon_a) \frac{J_1(|\mathbf{G} - \mathbf{G}'|r)}{|\mathbf{G} - \mathbf{G}'|r} \frac{\pi r^2}{\sqrt{3}\Lambda^2} \left(1 + e^{i(G_x - G'_x)\Lambda/2} e^{i(G_y - G'_y)\sqrt{3}\Lambda/2}\right), & \mathbf{G} \neq \mathbf{G}' \end{cases}. \quad (2.57)$$

Here, J_1 is the Bessel function of the first order.

In the grating region, the electric and magnetic fields are couple by the Maxwell's curl equations. Therefore, the transverse components (according to Eqs. 2.1) of them are written as

$$\partial_z E_x = k_0 H_y + \partial_x [(k_0 \varepsilon)^{-1} (\partial_x H_y - \partial_y H_x)], \quad (2.58a)$$

$$\partial_z E_y = -k_0 H_x + \partial_y [(k_0 \varepsilon)^{-1} (\partial_x H_y - \partial_y H_x)], \quad (2.58b)$$

$$\partial_z H_x = k_0 \varepsilon E_y + \partial_x [(k_0)^{-1} (\partial_x E_y - \partial_y E_x)], \quad (2.58c)$$

$$\partial_z H_y = -k_0 \varepsilon E_x + \partial_y [(k_0)^{-1} (\partial_x E_y - \partial_y E_x)], \quad (2.58d)$$

Eqs. (2.58) can be rearranged into matrix as before,

$$\partial_z \mathbf{E} = k_0 \begin{bmatrix} -\mathbf{K}_x [\varepsilon]^{-1} \mathbf{K}_y & \mathbf{I} + \mathbf{K}_x [\varepsilon]^{-1} \mathbf{K}_x \\ -\mathbf{I} - \mathbf{K}_y [\varepsilon]^{-1} \mathbf{K}_y & \mathbf{K}_y [\varepsilon]^{-1} \mathbf{K}_x \end{bmatrix} \mathbf{H} = k_0 \mathbf{P} \mathbf{H}, \quad (2.59a)$$

$$\partial_z \mathbf{H} = k_0 \begin{bmatrix} -\mathbf{K}_x \mathbf{K}_y & [\varepsilon] + \mathbf{K}_x^2 \\ -[\varepsilon] - \mathbf{K}_x^2 & \mathbf{K}_y \mathbf{K}_x \end{bmatrix} \mathbf{E} = k_0 \mathbf{Q} \mathbf{E}, \quad (2.59b)$$

Eliminating $\mathbf{H}$, we have eigenequation as

$$\partial_z^2 \mathbf{E} = k_0^2 \mathbf{P} \mathbf{Q} \mathbf{E}. \quad (2.60)$$

Therefore, the same idea can be employed by setting $\mathbf{A} = \mathbf{P} \mathbf{Q}$ that have been developed in previous sections. $\mathbf{\Gamma}$ is defined as the square root of the eigenvalues γ_m of $\mathbf{A}$ in diagonal matrix form. The modes of propagating electric field are expressed by the columns of $\mathbf{W}$ and $\mathbf{V}$ in the grating region, among which from the Eq. (2.59a) or (2.59b) can calculate the magnetic field modes. However, it is better to use

$$\mathbf{V} = -\mathbf{Q} \mathbf{W} \mathbf{\Gamma}^{-1}, \quad (2.61)$$

as the only requirement is to inverse the diagonal matrix for it.

By using the approach discussed in section 2.3, we combine the different layers of the structure.

Finally, the z-components of $\mathbf{R} = [\mathbf{R}_x \ \mathbf{R}_y \ \mathbf{R}_z]^T$ and $\mathbf{T} = [\mathbf{T}_x \ \mathbf{T}_y \ \mathbf{T}_z]^T$ must be considered by calculating the efficiencies. With the modes' orthogonality, we have

$$k_{Iz,n}R_{z,n} = k_{xn}R_{x,n} + k_{y,n}R_{y,n} , \quad (2.62a)$$

$$-k_{IIIz,n}T_{z,n} = k_{xn}T_{x,n} + k_{y,n}T_{y,n} . \quad (2.62b)$$

Finally, the field distributions of the device are calculated as before in a big matrix. The 3D $\boldsymbol{\Psi}$ matrix should contain three magnetic and electric field components, which means $\boldsymbol{\Psi} = [\mathbf{E}_x \ \mathbf{E}_y \ \mathbf{E}_z \ \mathbf{H}_x \ \mathbf{H}_y \ \mathbf{H}_z]^T$. $\mathbf{W}_z$ and $\mathbf{V}_z$ are defined for the added z-components. From Maxwell's Eqs. (2.1) and (2.2), we obtain

$$k_0\varepsilon E_z = \partial_x H_y - \partial_y H_x, \quad (2.63a)$$

$$k_0 H_z = \partial_x E_y - \partial_y E_x. \quad (2.63b)$$

from which we have

$$\mathbf{W}_z = [[\varepsilon]]^{-1}[-\mathbf{K}_y \ \mathbf{K}_x]\mathbf{V}, \quad (2.64a)$$

$$\mathbf{V}_z = [-\mathbf{K}_y \ \mathbf{K}_x]\mathbf{W}. \quad (2.64b)$$

Now, the $\mathbf{M}$ matrix for calculating the coefficients of field amplitude is expressed as

$$\mathbf{M} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ \mathbf{W}_z & -\mathbf{W}_z \\ \mathbf{V} & -\mathbf{V} \\ \mathbf{V}_z & \mathbf{V}_z \end{bmatrix}. \quad (2.65)$$

They are similar to these used in previous section 2.2.2. The introduction of $\Phi_y(y)$ is necessary due to the periodicity in y . Therefore, by using this algorithm, the fields at any point for the whole device can be calculated as

$$\Psi(x, y, z) = \Phi_x(x)\Phi_y(y)\mathbf{M}\Phi_z(z)\mathbf{C}. \quad (2.66)$$

The 2D RCWA algorithm will be verified in **Chapters 3 to 6**, where it is employed to sweep geometric parameters.

2.5 Conclusion

In this chapter, the RCWA algorithm has been developed for single-layer binary gratings, multilayer binary gratings and 2D gratings with under TE and TM polarized excitations. We developed Matlab codes to implement the RCWA algorithm such that we can calculate the transmission and reflection of metamaterials and PhCs. Compared with COMSOL, CST, and FDTD that need to define meshing, the RCWA algorithm is more efficient. In this thesis, the RCWA algorithm is employed to sweep parameters (geometric parameters, angles of incidence, wavelength, and frequency).

Chapter 3: All-dielectric active photonics driven by bound states in the continuum

3.1 Introduction

The theoretical investigation of dielectric cylinder resonators can be traced back to seminal analysis by Richtmyer in 1939 [147]. From then on, dielectric resonator has been extensively investigated for application on antennas at microwave frequencies [148-153]. Later, O' Brien and Pendry theoretically investigated high-index dielectric cylinders arranged periodically, showing $\varepsilon_{eff} < 0$ that is known as negative effective permittivity [154], which became one of essential methods for constructing negative effective index $n_{eff} < 0$ media. Within 20 years ago, the metallic SRRs, as the basic building blocks of metamaterials, were first proposed to present negative effective permeability $\mu_{eff} < 0$ at the microwave frequencies [155-160]. Both $n_{eff} < 0$ and $\mu_{eff} < 0$ at common range of frequency leads to the negative effective index $n_{eff} < 0$ metamaterials [155-161]. However, metals unfortunately show Ohmic (or heat) losses beyond the microwave frequencies, which once again sets requirement for exploring all-dielectric platforms to offer low-loss meta-optics and photonics. Most recently, the advances of meta-optics and photonics have revealed an unprecedented use of all dielectrics in optical metamaterials building blocks with high-index dielectrics that have readily emerged as an alternative approach to disrupt the lossy metal-based subwavelength photonics [162-182].

Several interesting physics phenomena in this field are driven by high- Q resonances, which is one of the most important parameters for evaluating the strength of light-matter interaction. The structures with high- Q factors offer a new route for strong wave localization at near fields that allow bio-/chemical sensors, optical filter, harmonic generations [177-182], and other optical devices to be realized. Most recently, the non-radiating BICs, demonstrating as spatial localization but coexisting with radiation continuum of free propagating waves, are attracting many research interests in nanoparticles and metasurfaces for the realization of many useful

functionalities including lasing and biosensing [77, 94-101, 183-190]. Initialized in quantum mechanics, the BIC phenomenon unprecedentedly developed in the fields of artificially metamaterials and PhCs due to their size-dependent wavelength tunability and arbitrary building blocks. So far, the BIC transforms into quasi-BIC, or supercavity, by introducing small losses into the system [183], where the resonant Q -factor (or resonance lifetime and resonance linewidth) becomes finite and measurable at the quasi-BIC conditions. Importantly, the BIC-inspired mechanism of wave localization makes it possible to realize high- Q resonances in metasurfaces that can be designed as pixelated dielectric metasurfaces for imaging-based molecular barcoding [98-100].

In this chapter, the physics of BICs are employed for achieving extremely high- Q factors in terahertz dielectric metasurfaces. The BICs in the quasi-state, known as supercavity with Q -factor larger than 250, is also experimentally demonstrated with the CW terahertz spectroscopy in frequency domain. With silicon (semiconductor) as metasurface building block, we show an active control of the supercavity with dynamical tunability with the optical pump-terahertz probe (OPTP) spectroscopy studies. The high- Q supercavity enables low-threshold (fluence of $10.16 \mu J/cm^2$) switching, where the recombination dynamics of the photo-generated carriers could be tailored at nanosecond timescale. Therefore, the photoconductivity of high-index semiconductors reveals an optimized platform for the dynamic control of high- Q resonances by tuning the pump fluence of external photoexcitation. This approach opens broad perspectives for designing active metamaterials and photonic devices towards filling the terahertz gap.

3.2 Bound states in the continuum and supercavity modes

For the photonics community, the non-radiative eigenmodes of a periodic membrane are referred as guided modes since they lie below light cone [45, 51]. In contrast to these guided

modes, modes located above the light cone generally couple to radiation continuum of free space. However, there are still modes above the light cone uncoupled from the free space. They are known as the BICs [77-93]. The existing body of literature distinguishes several mechanisms of BICs. The first one is *symmetry-protected BICs* [77, 81, 82, 90]. The simplest case of BICs is related to the Γ point in the first Brillouin zone, while the symmetry incompatibility between PhCs and incoming waves may also lead to BIC states at other high-symmetry points [45, 191]. The intuitive physical description of the symmetry-protected BICs at the Γ point is that odd modes are uncoupled from the free space plane waves propagating in the normal direction. However, the rigorous symmetry analysis involves less intuitive methods of the group theory. The second possibility is to form BICs at an *off- Γ point in PhC membrane* due to destructive interference between the leaky tails of propagating Fourier modes [77, 81, 82, 90]. This effect can be described almost analytically by account of Fourier expansion over a small number of plane waves (periodicity of PhCs). The third mechanism describes a *resonance-trapped BICs in metasurfaces* reported recently [97, 183]. It also occurs due to the destructive interference between tails of leaky modes, while we distinguish this mechanism since effects in PhCs and metamaterials have different descriptions. We recall that metasurfaces consist of resonant structural elements, which are responsible for the unusual properties of these structures. Unlike the PhC membranes, the metasurfaces require a large number of plane waves to reproduce a multipole resonance in the structural element correctly, which correspond to almost flat dispersion-less branch at the Γ point [185].

Although BICs are uncoupled to the free space, they are discrete states in continuum of leaky modes. Thus, a small variation of parameters turns BICs into a leaky mode with extremely high- Q factor, which is known as supercavity mode [183]. Moreover, the true BICs occur only in infinitely elongated systems [77], thus in most practical devices, all possible BICs turn to supercavity modes with high- Q factors. Even for the perfect infinite structures, we study

supercavity modes by detuning parameters from its ideal BIC conditions. In particular, tuning of incident angle scans the wave vector of the modes in a periodic structure by selecting the leaky mode with different Q -factors. Only for discrete values of incident angle, we observe a divergence of Q -factor due to BIC [82]. The resonant-trapped BICs in metasurfaces are less sensitive to the light direction because they are formed due to the local resonances, which can be excited by different plane waves and therefore they are related to flat bands on a band diagram [186]. However, the resonance-trapped BICs are affected by the geometrical parameters, in contrast to the symmetry protected BICs which do not depend on the structural geometry. In addition, the inevitable structure imperfectness due to the fabrication process could also break the spatial symmetry of the metasurface and turn the perfect BICs into supercavity modes with a finite Q -factor [187, 188].

3.3 Structure design

Figure 3-1. 2D metasurface design for terahertz supercavity mode with extreme high- Q resonances. (a) Top view, and (b) perspective view.

We consider a design of periodic dielectric metasurface that supports resonance-trapped BICs. The building block of the metasurface is a silicon cuboid with width W , length L and height H , as shown in **Figure 3-1**. The cuboids are arranged on a quartz substrate at the nodes of a square

lattice with the lattice constant Λ . Such metasurfaces can be manufactured by a wide range of fabrication techniques, and size scales because of their striped air-groove structure. High-index dielectric antennas are known to possess a rich family of resonances [147-153], even when they are made of silicon [189]. The working principle of our active all-dielectric device is schematically illustrated in **Figure 3-1(a)**, where the supercavity modes are excited by the terahertz radiation and are modulated by the external optical pump stimulus.

3.3.1 Numerical simulation

CST Microwave Studio frequency domain solver and time domain solver according to the requirements of analysis. In the frequency domain solver, unit cell boundary condition is applied for the model, and ports with 18 modes are set for the highest accuracy. Tetrahedral mesh should be chosen for frequency domain solver with the default mesh size, and higher mesh value will be required for extremely fine structure that will consume more memory as the price. The frequency domain solver provides a better resolution that can capture most of the fine features in the spectrum. In the time-domain solver, periodic boundary condition is applied for the unit cell model. Plane wave source and probes are needed to be set with the chosen polarization states according to the requirements. Hexahedral mesh should be chosen for time domain solver with the default mesh size, and higher mesh size value is required for finer structures. The time domain solver better reproduces experimental progress in the time domain THz-TDs system and the scan length is also tunable for the requirement of different resolutions.

The finite-element method (FEM) based COMSOL Multiphysics is also employed for transmission, reflection, and band structure calculations. For EM wave applications, the electromagnetic waves, frequency domain (emw) in radio frequency solver and the electromagnetic waves, frequency domain (ewfd) in wave optics under optics solver are

frequently used for simulations. COMSOL allows different physics to be couple to each other so that complex simulations, for example, harmonic emission from localized resonances, are sequentially calculated by adding an emw and/or ewfd solver after the localized resonances solved. In addition, COMSOL can deal with the complex lattice such as hexagonal and 3D lattice with periodic boundary conditions for each sides of the lattice, which is simpler for their band structure analysis.

In addition, the rigorous coupled wave analysis (RCWA) is employed for theoretical calculations of the scattering and propagation of waves though periodic PhC and metamaterial membranes. The RCWA is based on semi-analytical Fourier method where exact solutions of EM waves can be found for grating structures. The stepwise description for RCWA can be briefly summarized. First, the periodicity allows us to expand the dielectric functions and Maxwell's equations into the Fourier series. Next, the space is divided into three parts: superstrate, device and substrate and they are isotropic in three dimensions for simple consideration. The eigenmodes in the superstrate and substrate can be expressed analytically. The modes in the periodic device are found numerically by solving an eigenvalue problem for wave vector in the propagating direction. The amplitudes of incident waves are given as initial conditions and the amplitudes of the outgoing waves (including evanescent ones) are found from the Maxwell's boundary conditions similar as the scattering and transfer matrix techniques. The RCWA uncovers physics of the periodic PhCs and metamaterials by considering the total field excitation so that it enables calculations of each diffraction order (which is not explicit for CST and COMSOL), resonance frequency and radiation Q -factors. The eigenmodes and their dispersion (not band structure) can be obtained since the RCWA deals with eigenmode problems in Fourier space.

3.3.2 Numerical results

As shown in **Figure 3-2(a)**, all resonances shift to low frequency as the length of silicon resonators increases from 60 μm to 300 μm . At certain lengths, the sharp mode indicated by dashed black line demonstrates a vanishing nature, as shown in **Figure 3-2(a)** and the inset of **Figure 3-2(b)**. In addition, the Q -factor of these sharp modes tends to diverge which is a common attribute of BICs [77], as shown in **Figure 3-2(b)**. We observe two BIC regions that are labeled as BIC I at 0.58 THz with $L = 165 \mu\text{m}$ and BIC II around 0.39 THz with L approaching 300 μm . It is worth noticing that the BICs in PhC membranes are robust against the structural changes that preserve the spatial symmetry [188]. However, the scenario is different in metasurfaces. In the present case, the varying length of the cuboid L also preserves the spatial symmetry but the BIC I in our metasurface transitions into a high- Q mode, which confirms the difference between these two types of BIC.

The BIC I gets suppressed due to the existence of substrate in the fabricated device with significant Rayleigh diffractions (i.e. appearance or disappearance of diffracted orders into evanescent modes). We therefore focus our study on BIC II mode by adopting RCWA. Using this method, it is convenient to introduce an operator of normal component of the wave-vector $\hat{K}_z$, whose eigenstates are evanescent and propagating modes in the normal direction by considering the periodic media to be an infinite continuation of the metasurface. RCWA yields amplitudes of the periodic media eigenstates as a function of frequency. In the metasurface with the length L below 300 μm and $W = 210 \mu\text{m}$, the supercavity mode is explained by the destructive interference between a propagating mode and an evanescent solution with imaginary K_z . The analysis of eigenmode amplitudes makes it possible to evaluate Q -factor directly (**Figure 3-2(b)**), because in the vicinity of resonance mode the amplitudes are described by the Lorentz function, in contrast to the transmission spectra with Fano resonances as the result of the mode interference. The BIC mode manifests itself in the transmission spectra as a pronounced Fano resonance, which has an asymmetric line shape [84, 190, 191]. We

extracted the resonance Q -factors from the transmission spectra by using the Fano formula, given by $T_{Fano} = \left| a_1 + ia_2 + \frac{b}{\omega - \omega_0 + i\gamma} \right|^2$, where a_1 , a_2 and b are constant real numbers; ω_0 is the central resonant frequency; γ is the overall damping rate of the resonance. The experimental Q -factor was then determined by $Q = \omega_0/2\gamma$ [163, 177, 180], which show similar results.

Figure 3-2. BICs and supercavity resonance. (a) Map of transmission spectra by sweeping the cuboid length from 60 μm to 300 μm , where the width (210 μm) and the height (200 μm) are kept constant. The terahertz wave impinges at normal incidence. The low frequency mode is marked by black dashed curve. Two BIC regions are indicated on the selected low frequency

mode. **(b)** Evolution of Q -factor at the low frequency mode of the metasurface by changing the cuboid length. Inset: the disappearance of transmission mode at BIC I at $L = 165 \mu\text{m}$. **(c)** Angle-resolved transmission spectra (left panel) and band diagram (right panel) of the silicon resonator in square lattice. The band structures calculated by COMSOL Multiphysics (red line) reliably reproduces the one obtained by the CST microwave studio (dots). **(d)** The corresponding electric and magnetic field profile for the TE-like eigenmodes at the Γ -point with frequency of 0.41 THz. The incident wave is polarized along x axis in **(a)** and **(b)**. The light line in **(c)** is labelled as dashed black line.

The wavevector (k_y) dependent transmission spectra (left panel) and band diagram (right panel) of the structure with $L = 270 \mu\text{m}$ and $W = 210 \mu\text{m}$ are plotted in **Figure 3-2(c)**. The band structure is calculated using the finite element method in COMSOL Multiphysics (red solid lines) and the results are reliably reproduced by using the eigenmode solver from CST microwave studio (red dots). By comparing the two panels in 3-2(c), the angle-resolved transmission spectra show consistent behavior of eigenmodes in the band structure, where the existence of eigenmodes imply that the terahertz wave can propagate and transmit through the periodic membrane. The resonance frequency and linewidth of the supercavity mode at 0.41 THz (in the vicinity of BIC II) are less sensitive to the symmetry-breaking perturbations near the Γ point (highlighted by the circles) but depend strongly on the cavity geometry. Therefore, we verify that the proposed system supports *resonance-trapped BICs*. **Figure 3-2(d)** shows the distributions of the electric and magnetic field in the cavity at the Γ point of the band highlighted by the circles. The magnetic field distribution exhibits a pair of magnetic dipoles along the z -axis oscillating out of phase. We note that unlike spherical or cylindrical dielectric resonators, a rigorous classification of modes of a dielectric cuboid do not exist [151-153]. Following the notation of ref. [152] one can use TE_{211}^z nomenclature to describe the observed

modes in cuboids. Thus, we restrict ourselves to mode description in **Figure 3-2(d)** and leave cuboid mode classification beyond the scope of this work.

3.3.3 Parameter optimization

To clearly show the dependence of the supercavity modes on different geometry parameters, we discuss the simulated data below.

Figure 3-3. The transmission map as function of the resonator width W , while the length and width are kept constant at $270\ \mu\text{m}$ and $210\ \mu\text{m}$, respectively. The dashed cyan line labels the 1st order diffraction where the supercavity mode shows at $W = 130\ \mu\text{m}$. (a) air cladding and (b) quartz as substrate (real sample scenario).

a) Effect of width (W) on BIC

To quantify the effect of width on BIC, we performed extensive numerical simulation by varying the width of resonators, where the length is fixed at $270\ \mu\text{m}$ and the height is fixed at $210\ \mu\text{m}$. The transmission maps are shown in **Figure 3-3(a)** without substrate and **3-3(b)** with quartz as substrate. From these two maps, we can conclude:

- i. The supercavity mode shifts to the lower frequency as the width of resonator increases.

- ii. The linewidth of the supercavity mode (i.e. Q -factor of resonance) does not change with width (W) of the structure.
- iii. To avoid the non-zero Rayleigh diffraction (radiation losses at 0.47 THz due to periodic quartz substrate), the width of structure should be larger than 130 μm , as shown in **Figure 3-3(b)**. Therefore, the chosen width ($W = 210 \mu\text{m}$) of our structure ensures that supercavity mode is not suppressed by the Rayleigh diffraction. This guarantees that the supercavity modes can be experimentally measured.

b) Effect of H on BIC

The height-dependent transmission map is shown in **Figure 3-4**. The simulation results suggest:

- i. The supercavity mode shifts to the lower frequency as the height of resonator increases.
- ii. The linewidth of supercavity mode does not dramatically change as the height of resonator increases.
- iii. The 1st order diffraction lies at 0.47 THz once quartz is taken as substrate, as shown in **Figure 3-4(b)**. Therefore, the resonator's height should be larger than 60 μm to avoid the suppression of supercavity mode. The selected geometric parameter with a height of 200 μm is optimized for ease of fabrication and measurements.

Therefore, the linewidth of resonances, or Q -factor, are not obviously dependent on the width (W) and height (H) of the resonators. Therefore, we restrict our discussion on the different geometric length (L) while keeping the width (W) and height (H) of the resonators unchanged. Particularly, the width ($W = 210 \mu\text{m}$) and height ($H = 200 \mu\text{m}$) are optimized to avoid the 1st order diffraction at frequency of BIC-II, and meanwhile guarantee the feasibility of fabrication

and experiments of the samples. We have added these discussions to the Supplemental materials in the revised manuscript.

Figure 3-4. The transmission map as function of the resonator height H , while the length and width are kept as 270 μm and 210 μm unchanged. The dashed cyan line labels the 1st order diffraction where the supercavity mode shows at $H = 60 \mu\text{m}$. (a) air cladding and (b) quartz as substrate.

3.4 Experimental observation of terahertz supercavity modes

3.4.1 Sample fabrication

Through this thesis, the samples were fabricated using high-resistivity silicon ($>10000 \Omega\cdot\text{cm}$) due to its low loss and low dispersion at terahertz frequencies. The thickness of designed all-dielectric metasurfaces is usually ranging from 100 microns to 1000 microns. The relatively large size of resonators operating in the terahertz band requires a different fabrication method from those operating in the visible and IR spectra [192]. In particular, such a thick silicon layer on insulator (SOI) could not be grown by chemical vapor deposition (CVD) and thus, it would be virtually impossible to fabricate these resonators by a conventional one-step reactive ion etching (RIE). Here, we followed a five-step fabrication procedure:

- (1) Deposition of SiO₂. A 2 μm SiO₂ is deposited on the cleaned high-resistivity silicon (>10000 Ω·cm) wafer with thickness of 200 μm by the plasma-enhanced chemical vapor deposition (PECVD), where the selectivity of the etching gas ions on Si and SiO₂ determines the deposition thickness of the SiO₂ layer. The SiO₂ is mask layer during the process of silicon etching.
- (2) Spin-coating photoresist on the SiO₂-Si hybrid wafer. The AZ 5214E photoresist is spin coated on the SiO₂-Si hybrid wafer with spin speed of 4000 rpm for 40 s with acceleration deceleration time is 3 s and deceleration time is 5 s, which make sure the thickness of photoresist is larger than 1.5 μm. To solidify the photoresist, the photoresist-coated samples are baking for 2 mins on hot-plate with temperature of 105 °C.
- (3) Patterning of photoresist spin-coated silicon wafer with UV photolithography. The hybrid photoresist-coated SiO₂-on-silicon wafer is patterned by conventional UV photolithography on SiO₂. After photolithography, the photoresist is lifted off by using AZ 422 for about 1 minute to remove the UV illuminated photoresist.
- (4) Gluing the silicon wafer to a quartz substrate with UV curable adhesive (NOA 85, $n = 1.48$). The hybrid silicon dioxide-on-silicon wafer with patterns is then directly bonded to a 1-mm quartz substrate with a thin layer of spin-coated UV curable polymer optical adhesive (Norland Optical Adhesive 85) and exposure to UV light (2.5 W/cm²) for 10 mins.
- (5) Etching of silicon-on-quartz composite with deep reactive ion etching (DRIE) process. After bonding, the SiO₂ is removed by mixed gases of CHF₃ and CF₄ and the remaining pattern is kept as a protection mask for subsequent silicon etching. The silicon wafer is etched by the DRIE (deep reactive ion etching technique, Oxford Estrelas). Each cycle of the Bosch process consists of sidewall passivation (C₄F₈) and etching (SF₆) steps

with deposition of 5 s and etching of 15 s. In the deposition step, the C₄F₈ gas (85 sccm) is utilized with 600 W ICP power at 35 mTorr pressure. During the etching step, a mixture of SF₆ etching step, a mixture of S₆ (130 sccm) and O₂ (13 sccm) is applied with 600 W ICP power and 30 W bias power, at 35 mTorr pressure. This process cycle is then repeated until the silicon is completely removed. Solid silicon metasurface arrays are kept attached to the quartz substrate.

3.4.2 Materials characterization with THz-TDS

The transmitted time-domain terahertz pulse for 200-μm silicon (Orientation <100>) and 1-mm quartz (z-cut) are plotted in **Figure 3-5**. Compared to the reference signal (terahertz pulse for dry nitrogen atmosphere), transmitted peak field decreases due to the materials' reflections at the interfaces and absorption in materials even though the absorption is small. Silicon has the largest refractive index among three, so it has lowest transmitted terahertz pulse with the fixed initial position. Terahertz pulses of silicon and quartz are delayed respect to nitrogen. Quartz has the largest delay since the thickness is 5 times of silicon. The two materials under used are optically thick samples, which indicates the terahertz signal drops zero before echo comes out. With the time-domain pulses and accurate sample thicknesses, the refractive indices are calculated by solving $\tilde{T}(\omega) = \frac{2\tilde{n}(\tilde{n}_{sup} + \tilde{n}_{sub})}{(\tilde{n} + \tilde{n}_{sup})(\tilde{n} + \tilde{n}_{sub})} \cdot e^{(-i(\tilde{n} - \tilde{n}_{sub})\frac{\omega d}{c})} \cdot FP(\omega)$, where ω and c are the angular frequency and speed of light in a vacuum [4, 5]. The complex refractive index $\tilde{n}$ is the one to be solved, and $\tilde{T}$ is the complex transmission that is calculated by fast Fourier transform. $FP(\omega)$ is the frequency dependent contribution of Fabry-Perot reflections, and here it is one since silicon and quartz film are optically thick samples with thickness of d . The wafers are cladded by Nitrogen so the complex refractive indices $\tilde{n}_{sup}$ and $\tilde{n}_{sub}$ are taken as the refractive index of air. As shown in **Figure 3-5**, both silicon and quartz have negligible absorption and dispersion-free characteristic in the frequency regime of interest. These

experimentally extracted values are taken for numerical simulations and theoretical calculations in this thesis.

Figure 3-5. Experimental study the terahertz properties of 200 μm silicon (orientation $\langle 100 \rangle$) and 1 mm quartz (z-cut). **(a)** Transmitted time-domain terahertz pulses for dry nitrogen, silicon and quartz. **(b)** Corresponding refractive indexes for silicon and quartz with reference of nitrogen.

3.4.3 CW Terahertz spectroscopy

Even thick substrate was employed to do longer scan measurement, the terahertz-TDS is still limited by the resolution at the gigahertz range. Therefore, high-resolution terahertz measurements were also done by employing a commercially available terahertz system (TeraScan 1550 from Toptica) [28]. It is a CW-based terahertz spectroscopy system with high frequency resolution down to 10 MHz, which has combined coherent generation and detection of terahertz radiation in frequency-domain using fiber coupled photoconductive antennas (InGaAs PCAs). Two distributed feedback (DFB) lasers at adjacent frequencies illuminate the photo mixer antennas to generate terahertz radiation and detect terahertz signal by measuring the photocurrent at the detector PCA. To resolve the spectral resolution to 10 MHz, 100 ms integration time is needed to take one data. The measurements were done at room temperature and in the dry nitrogen atmosphere to nullify the effect due to water vapor absorption.

3.4.4 Experimental results

Figure 3-6(a) shows the theoretical transmission spectra by varying the resonator length from 230 μm to 270 μm with step size of 10 μm , while the width $W = 210 \mu\text{m}$ is kept unchanged. Measured terahertz refractive indexes of silicon ($n = 3.48$) and quartz substrate ($n_{sub} = 2.14$) were used to perform the numerical simulations. Overall, the resonances show red-shift and the Q -factors increase as the resonator length increases. A non-zero (i, j) Rayleigh diffraction channel opens up at the frequency evaluated by $f = \frac{c}{\Lambda n_{sub}} \sqrt{i^2 + j^2}$, where c is vacuum light speed, Λ is the lattice constant, n_{sub} is refractive index of quartz substrate [50]. Additional scattering channels result in decrease of Q -factor and appearance as a suppression feature in the zero-order transmission spectra [193]. In our devices, this feature is observed at 0.47 THz (first order diffraction, $i = \pm 1, j = 0$), as shown in **Figure 3-6(a)** that is labeled as a dashed black line. We restrict our attention towards the low-frequency resonances below 0.47 THz for $L \geq 215 \mu\text{m}$ since they have relatively larger amplitude for identification and accurate measurement. To experimentally probe the high- Q resonance in the supercavity, we fabricated samples with the identical parameters as used in numerical calculations. The transmission spectra of each sample were measured using a CW terahertz spectroscopy (TeraScan 1550) with high resolution for high- Q resonance measurements (see Methods for details). As shown in **Figure 3-6(b)**, the measured spectra show excellent agreement with the numerical calculations. The supercavity resonance mode below 0.47 THz reveals red-shift, and the corresponding Q -factors gradually increase from 42 to 250 when L increases from 230 μm to 270 μm . The diffraction channel is also clearly observed at 0.47 THz indicated by a dashed black line as shown in **Figure 3-6(b)**, above which the transmission amplitude gets suppressed. We note that the accurate frequencies of diffraction kinks in the experiments reveal slight deviation due to the non-uniform thicknesses of UV curable adhesive in the samples.

Figure 3-6. Experimental measurement of the high- Q supercavity mode in all-dielectric metadvice. **(a)** Transmission spectra of the proposed device at normal incidence by changing length of the cuboid resonator L from 230 μm to 270 μm with a step size of 10 μm in numerical calculations. The dashed line indicates the frequency where the first order diffraction occurs. **(b)** Corresponding transmission spectra from measurements with the same parameters as simulations. **(c)** The map of numerical transmission spectra for real devices by changing the resonator length L . The horizontal dashed line indicates the emergence of the first order diffraction, and the vertical dashed line indicates the geometric length where the supercavity mode emerges. **(d)** Comparison of Q -factors for the ideal case with air cladding (black curve), real case with quartz substrate (red curve), and experimentally captured Q -factors from measurements (magenta dots).

A full map of transmission spectra by changing the length of the resonator from 60 μm to 300 μm is shown in **Figure 3-6(c)**. We observe the suppression of zero-order transmission mode above the frequency of non-zero diffraction channel at 0.47 THz as shown by the horizontal dashed black line. Therefore, the BIC I region disappears due to the excitation of high-order

diffraction modes in samples with quartz substrate. The supercavity resonances reappear when the resonator length exceeds 215 μm , as illustrated in **Figure 3-6(c)** (vertical black dashed line). Above a specific resonator geometry, the numerically calculated and the experimentally measured supercavity resonances are plotted as red solid line and magenta dots in **Figure 3-6(c)**, respectively. Following the resonance evolution trajectory, we extracted the Q -factors of numerical calculations (ideal case with air cladding, and real case with quartz substrate) and measured spectra, as plotted in **Figure 3-6(d)**. Overall, the measured resonance Q -factors show good agreement with the numerical simulations. The Q -factors for ideal case is significantly larger than that of real case but the maximum of measured Q -factor reaches 250 that is the highest value for THz dielectric metasurfaces. This also indicates the transition from BIC to supercavity mode due to the existence of substrate that introduces an asymmetric mode profile (additional scattering losses) within the structure. It should be noted that the Q -factor diverges for both ideal and real devices as the length of the silicon resonators approaches 300 μm , which provides further evidence of the existence of resonance-trapped BICs.

3.5 Active control of terahertz supercavity modes

3.5.1 ZnTe-based optical-pump terahertz probe spectroscopy

THz-TDS system was employed to characterize the response of metamaterial samples through this thesis. Passive transmission and dynamic performance of the all-dielectric metamaterials were performed using the optical pump-terahertz probe (OPTP) spectroscopy setup. A near-infrared laser beam (Ti: sapphire oscillating laser system, 35 fs, 6 mJ per pulse at 800 nm with 1 kHz repetition rate) was coherently split into three parts: external pump source, pump beam for generation of terahertz radiation and detection beam for terahertz detection. To capture the active modulation of terahertz transmission, the transmitted terahertz time-domain signal through the samples were recorded with a scan length of 100 ps. Further, the optical pump

fluence is tuned by a neutral density filter to capture the modulated time-domain signal. To avoid the Fabry-Perot (FP) resonance, a thick quartz (10 mm, identical to the substrate) was attached to the sample (200 μm silicon on 1 mm quartz substrate). Therefore, the substrate becomes 11 mm and terahertz echo signal (FP resonances) are highly delayed after the high- Q resonance (long lasting oscillations in time domain) reaches the steady state. The time domain signals were transformed to frequency domain and normalized by using an identical bare quartz substrate as the reference by $|\tilde{T}(\omega)| = |\tilde{E}_s(\omega)/\tilde{E}_R(\omega)|$, where $\tilde{E}_s(\omega)$ and $\tilde{E}_R(\omega)$ are the spectra of sample and reference after Fourier transform, respectively. For the measurements of free carrier dynamics, we set the synchronization position of terahertz probe and optical pump at the maximum of time-domain terahertz pulse and monitored the time-varied terahertz amplitude at this point by changing the delay time of pump pulse.

3.5.2 Dynamic supercavity modulations

As one of the most promising applications, active modulator with on-demand optical properties is a key technology in wave-front engineering, near-field control of EM radiation, and multi-channel optical data processing [106]. In the terahertz regime, optical pump and terahertz probe (OPTP) technique has been widely adopted to investigate all-optical active metadevices [124, 125, 182, 193-196]. Typically, these devices consist of an active layer made of semiconductor such as Si, Ge, or GaAs, in addition to a metal-based resonator array. In our device, the silicon resonators themselves act as the active medium due to photo-generated charge carriers when pumped by an external optical stimulus with photon energy (1.55 eV) larger than the bandgap of silicon (1.1 eV). The optically induced free carriers enable the change of conductivity on the surface of silicon resonators with a penetration depth of about 10 μm [193]. Following the OPTP approach, we have experimentally demonstrated an all-optical active modulation of the supercavity mode (sample with length of 230 μm , $Q = 42.36$) where the modulation depth is controlled by applying a femtosecond pulsed laser stimulus (@800 nm wavelength, 1 KHz

repetition, 100 fs pulse width). As shown in **Figure 3-7(a)**, the supercavity mode is continuously modulated in terms of resonance intensity as well as Q -factor by gradually tuning the photoexcitation pump fluence. The resonance peak (at 0.46 THz) as well as the two resonance dips (at 0.43 THz and 0.53 THz) are completely switched off rendering a flat spectral response at an optical pump fluence of $63.5 \mu\text{J}/\text{cm}^2$ (power of 50 mW). During this modulation process, two interesting events appear (a) the resonance peak of the supercavity mode at 0.46 THz gradually diminishes and eventually quenches at a pump fluence of $10.16 \mu\text{J}/\text{cm}^2$ (power of 8 mW), and (b) the broadband (0.3-0.6 THz) terahertz transmission spectrum becomes flat quenching the low Q -factor modes as the pump fluence becomes larger than $10.16 \mu\text{J}/\text{cm}^2$. Upon photoexcitation, the strong damping due to the photo-induced free charge carriers prohibits the tight confinement of resonant field inside the silicon resonators. As the pump fluence is further increased, large number of photo-carriers dominantly damps and broadens resonances such as Mie modes. Therefore, the resonant transmission dips (at 0.43 THz and 0.53 THz) gradually increase and disappear as a flat spectrum beyond pump fluence of $63.5 \mu\text{J}/\text{cm}^2$. In short, the two-stage modulation process occurs due to the change in the concentration of excited photo-carriers with the increase in pump fluence. First, the ultrasensitive supercavity mode damps out due to the injection of photocarriers leading to the broadening of the resonance linewidth. The damping of the high- Q supercavity mode occurs at extremely low fluence of $10.16 \mu\text{J}/\text{cm}^2$, at which the loss is large enough to completely quench the strongly resonant mode. Further, the release of supercavity resonant energy leads to the overall increase of transmission amplitude at pump fluence larger than $10.16 \mu\text{J}/\text{cm}^2$.

The two-stage modulation of spectra can also be observed from the measured terahertz time-domain signals. Since photons are tightly confined inside the resonators at the supercavity mode without dominant loss channel, the oscillations in the terahertz time-domain pulse lasts longer than 100 ps as observed in **Figure 3-7(b)**. Once a loss channel is introduced, the

oscillation amplitude of supercavity mode rapidly damps and thus ringing amplitude at longer time duration reduces significantly. The contrast is clearly captured by introducing the pump stimulus (pump fluence of $63.5 \mu\text{J}/\text{cm}^2$) as shown in the inset plot of **Figure 3-7(b)**, where a rapid decay of oscillation occurs within 10 ps due to the excitation of large density of photocarriers. The evolution of time-domain pulses versus pump fluence is visualized clearly within 20 ps in **Figure 3-7(b)**. We have divided the time-domain pulse into two regions with gray and cyan background with a boundary at a time instant of 4 ps. The gradual amplitude damping in the gray region accounts for the modulation of supercavity mode intensity and Q -factor, and the resonance mode (resonance peak at around 0.46 THz) vanishes at a fluence of $10.16 \mu\text{J}/\text{cm}^2$. On the other hand, the release of confined photons from the supercavity mode leads to the restoration of energy back into the main terahertz pulse as shown in the cyan region, where we observe the increase in amplitude of time-domain pulse as the pump fluence increases. This accounts for the gradual increase of broadband transmission amplitude at larger pump fluences in frequency domain as shown in **Figure 3-7(a)**.

Figure 3-7. Photoexcitation dependent dynamic modulation of the supercavity resonance. **(a)** Experimentally measured transmission spectra showing the continuous modulation of supercavity mode by tuning the pump fluence. **(b)** Corresponding time-domain pulse modulation by varying pump fluence within 20 ps. Two regions are indicated to explain the

fluence dependent mode evolution behaviors. Inset: Full length of time-domain pulses for 100 ps with and without optical pump.

Figure 3-8. Temporal evolution of the supercavity resonance. **(a)** Measured differential transmission of terahertz time-domain amplitude at 4.8 ps (blue triangle in **Figure 3-7(b)**) as a function of delay time of pump pulse. The relaxation dynamics is scanned for 2650 ps with a femtosecond pump pulse (@800 nm, 1.55 eV, silicon band gap ~ 1.14 eV). The cyan curve is the exponential fitting of the carrier-relaxation. Insets show the schematic illustration of carrier concentration at various time delays. **(b)** Measured transient frequency-domain transmission spectra of the supercavity device at various time delays.

In addition to the fluence dependent supercavity mode evolution, the transient dynamics reveals the time-resolved evolution of the supercavity mode. Since the modulation stems from generated photocarriers, we probed the dynamics of charge carriers in intrinsic silicon with the optical pump fluence of $63.5 \mu\text{J}/\text{cm}^2$ as shown in **Figure 3-8(a)**. Here, the differential transmission $-\Delta T/T_0$ is directly proportional to density of photocarriers, where $\Delta T = T(t) - T_0$, and $T(t)$ is the time-domain transmission amplitude through the sample at a given transient (t), and T_0 is the steady state amplitude (blue triangle in **Figure 3-7(b)**) of the sample in the absence of optical excitation. The transient $-\Delta T/T_0$ spectrum shows the carrier dynamics

between the valence and conduction bands under optical pump, whose relaxation dynamics can be fitted by a single exponential decay function. The fitting equation is $-\Delta T/T_0 = A_0 + A_1 e^{-(t-t_0)/\tau}$, where A_0 and A_1 are constants, t_0 corresponds to the time when $-\Delta T/T_0$ reaches the maximum, and τ is the decay constant. Most of carriers lie in valence band (VB) before the arrival of the pump pulses. Conduction band (CB) has few residual carriers due to thermal effect from the laser pulse (repetition rate of 1 kHz). The differential transmission ($-\Delta T/T_0$) dramatically increases within 12.68 ps due to the large amount of photocarriers pumped into CB. The photocarriers lead to the modulation of transmission amplitude and thus the supercavity resonance spectrum, which is completely switched off at 12.68 ps as shown by the red curve in **Figure 3-8(b)**. The photocarriers gradually recombine following an exponential decay with increasing time delay. In order to probe the transient evolution of the supercavity mode, we present the measured transmission spectra at different temporal instants (995.35, 1661.81, and 2595.79 ps) in **Figure 3-8(b)**, where we clearly observe the gradual recovery of the supercavity mode. At time instant of 2595.79 ps, the resonance mode almost recovers back to the original state. Thus, we consider 2.6 ns as the recovery time of the metadvice, which enables a sub-gigahertz switching speed. This switching speed could be further improved by several approaches, such as by adopting ion-implanted silicon, direct band-gap semiconductors (GaAs), and/or intra-band effects in semiconductors [123, 125, 197].

3.5.3 Pump fluence dependent dynamics and transmission spectra

Figure 3-9(a) shows the negative differential transmission $-\Delta T/T_0$ under different optical pump fluences. Compared to **Figure 3-7**, **Figure 3-9** shows more pump fluences and all the dynamics for each pump fluence. The black curves present the fittings for different dynamics under different pump pulses. The delay time constants are: 328 ± 10 ps, 435 ± 8 ps, 422 ± 4 ps, 468 ± 3.7 ps, 565 ± 3.6 ps, 704 ± 3 ps, 855 ± 3 ps, 1066 ± 4 ps, 1219 ± 5 ps, 2182 ± 17 ps as pump fluences increase from $1.27 \mu\text{J}/\text{cm}^2$ to $63.5 \mu\text{J}/\text{cm}^2$. It's obviously demonstrated that the

relaxation time is proportional to the pump fluence, which implies that the relaxation time is longer as the pump fluence increasing, and the relaxation becomes faster as the pump fluence getting smaller. Therefore, it is the trade-off between the dynamic duration and transmitted terahertz intensity that could be taken into consideration for real applications, as shown by frequency-domain spectra in **Figure 3-9(b)**.

Figure 3-9. The dynamic evolution (a) and corresponding transmission spectra (b) of optically pumped device under different pump fluences.

3.6 Conclusion

In summary, we have experimentally demonstrated an active control of all-dielectric terahertz metasurfaces that support high- Q supercavity resonance mode in the vicinity of the BICs. Two BIC regions emerge by tailoring the geometrical length of the silicon resonators, which are shown as the *resonance-trapped BICs*. Further, the dynamic switching and modulation of the all-dielectric metadvice were shown at extremely low fluence of pump light. In addition, a temporal spectral evolution of the supercavity resonance show sub-gigahertz switching speed of our all-optical active metadvice. Our findings open a novel avenue for an active control of

all-dielectric BICs based metasurfaces that would enable design of active terahertz on-chip, ultrafast, low-loss components and devices such as efficient modulators, filters, and biosensors.

Chapter 4: Guided-mode resonances in dielectric terahertz metasurfaces

4.1 Introduction

The resonance phenomena in photonics allow for strong localization of EM waves that is essential for numerous applications [77, 145, 164, 165, 170, 173, 198], such as narrowband filtering [199], out-of-plane wave coupling [200], chemical and biological sensing [201], lasing [97, 202], harmonic generation [180, 203-206], Raman scattering [207], and photovoltaics [208]. The important parameters that describe a resonance feature are its intensity and spectral linewidth. For most practical applications, resonances with strong intensity and narrow linewidth are desirable. Higher resonance intensity provides better signal to noise ratio, while narrower linewidth signifies larger field confinement. However, most of the resonances are constrained by the trade-off between resonance intensity and linewidth [208]. This limits the possibility of independent tailoring of resonance features at will. On the contrary, guided mode resonance (GMR) can provide arbitrary resonance intensity and linewidth through geometrical design and selection of materials [199]. Due to this versatile nature of GMRs, they have found wide range of applications, including extremely high- Q filters, ultra-broadband reflectors, wavelength selective polarizers, and beam splitters [199, 210-221]. The GMR filter primarily comprises of a diffractive grating and an in-plane waveguide. The grating diffracts the incident light and couples it into the waveguide, which propagates as a guided mode. However, this guided mode is designed to be leaky, which then interferes with the free space propagating EM wave to give rise to the GMRs. Through the selection of material, grating design, dielectric layer thickness, and angle of incidence, GMRs can provide a wide range of spectral features. Currently, the exploration of GMRs is limited to optical and radio frequency regions of the EM spectrum. However, terahertz technologies are attracting a lot of attention to cater to the challenges of meeting ever-increasing demand for high-speed wireless communications [32].

Terahertz GMR devices could play a crucial role in communication applications due to its capability for constructing high- Q filters, polarization selective beam splitters, differentiators, integrators, and wavelength division (de)multiplexers [199]. Earlier reports on terahertz GMRs were realized through 1D grating elements on quartz substrate [222] and periodic metallic patterns on cyclo-olefin substrates [223]. Here, we experimentally demonstrate silicon-based all-dielectric metasurfaces that support GMRs at THz frequencies. The 2D metasurface, building block with periodic array of subwavelength silicon microstructures, simultaneously acts as the diffraction grating as well as the slab waveguide and hence enables the observation of GMRs. At oblique incidence, two frequency detuned GMRs are observed, which arises from two counterpropagating modes in the slab waveguide. However, at normal incidence, the coupling of these two GMRs leads to a symmetry-protected BIC with infinite Q -factor. A detailed investigation of GMRs as functions of the geometrical parameters of the silicon microstructure and the angle of incidence are also presented in this work.

4.2 Guided-mode resonances

GMRs are widely believed as a resonance phenomenon arising from Wood's anomaly that refers to the rapid variations in the reflected and/or transmitted diffraction orders from corrugated gratings [224]. In 1941, Fano distinguished two principal types of Wood's anomalies [225]: the first one is known as Rayleigh anomaly that refers to the appearance or disappearance of diffracted orders into evanescent modes (surface waves), the second one is the diffuse anomaly by "a forced resonance" related to the leaky waves supported by the grating. Since then, there has been an intense investigation on this resonant anomaly based on the concept of *leaky mode resonance* or the *guided-mode resonances* [199].

In the present case, the silicon grating itself acts as waveguide layer. As a result, the averaged refractive index of the grating is given by $\varepsilon_g = f\varepsilon_{Si} + (1 - f)\varepsilon_a$ [226, 227], where $\varepsilon_a = 1$ is the permittivity of air, $\varepsilon_{Si} = 12.11$ is the permittivity of silicon, and f is the filling factor given

by the fraction of the area of a unit cell occupied by silicon resonators. The silicon grating layer is cladded by air as superstrate and quartz substrate ($n_{sub} = 2.14$). Therefore, the refractive index of waveguide layer ($n_g = \sqrt{\epsilon_g} = 2.83$) is larger than the refractive indices of both the cladding layers and hence satisfies the TIR condition required for guiding of the incident EM wave. According to ray tracing concept, the propagating wavevector in the effective waveguide slab is given by $\beta = n_{eff}k_0 = k_0n_g\sin(\theta)$, where k_0 is vacuum wavevector, n_{eff} the effective refractive index of waveguide, θ is the angle of incidence (or reflection) at the interface of slab waveguide and cladding layers. Since the waveguide is formed by patterned silicon resonators array, the diffraction of grating is governed by the grating equation $n_g\sin(\theta_m) = n_a\sin(\theta_{inc}) - m\frac{\lambda}{\Lambda}$, where θ_m is the m^{th} diffraction angle, n_a is the refractive index of the air, θ_{inc} is the angle of incidence, λ is the diffraction wavelength and Λ is the grating period. By combining the ray tracing equation and grating equation, we have the effective refractive index of the grating waveguide as $n_{eff} = n_a\sin(\theta_{inc}) - m\frac{\lambda}{\Lambda}$. Recall the TIR condition ($\max[n_a, n_{sub}] < n_{eff} < n_g$), we have equation describing the regions of resonance for guided-mode resonance as $\max[n_a, n_{sub}] < n_a\sin(\theta_{inc}) - m\frac{\lambda}{\Lambda} < n_g$. This expression allows the definition of parametric regions, within which the GMRs occur. The upper boundary of the GMRs (left-hand side of inequality) is $\frac{n_a\sin(\theta_{inc}) \pm \max[n_a, n_{sub}]}{m}$, $m = \pm 1$, and the low boundary of the GMRs (right-hand side of inequality) is $\frac{n_a\sin(\theta_{inc}) \pm n_g}{m}$, $m = \pm 1$. At the intersection of two GMR regions, a double Rayleigh anomaly occurs, where the resonances are degenerated at $\theta_{inc} = 0^\circ$ that corresponds to a center wavelength as $\frac{\lambda_c}{\Lambda} = \frac{n_2 \pm \max[n_a, n_{sub}]}{2|m|}$.

4.3 Metasurface building blocks and experimental measurements

The unit cell is a silicon cuboid resonator with length (L) of $270\ \mu\text{m}$ in x -direction, width of (W) $210\ \mu\text{m}$ in y -direction, and height (H) of $200\ \mu\text{m}$ in z -direction sitting in a square lattice with period $\Lambda = 300\ \mu\text{m}$, as shown in **Figures 4-1(a) and 4-2(b)**. The silicon ($n_{\text{Si}} = 3.48$) cuboid resonators are fabricated on a quartz substrate ($n_{\text{sub}} = 2.14$). High-resistivity silicon ($\rho > 10000\ \Omega\cdot\text{cm}$) was chosen, due to its low loss and low dispersion characteristics at terahertz frequencies, as discussed in chapter 3.

Figure 4-1. Design of terahertz all-dielectric metasurface for excitation of guided mode resonances (GMRs). (a) Perspective view and (b) Top view of the SEM images of the fabricated metasurface, respectively. (c) Photonic dispersion curves of the guided modes of the thin film waveguide. (d) Formation of leaky mode above light cone from the band folding of two guided modes from nearest neighbor Brillouin zones. (e) Inset showing the anti-crossing (blue) and

cross-over (red) behavior of two eigenmodes, approaching each other that signifies strong coupling and weak coupling regimes, respectively.

The SEM images of the fabricated metasurface are shown in **Figure 4-1(a)** (perspective view) and **4-1(b)** (top view), respectively. The 2D array of silicon cuboid resonators acts as a grating and more importantly, the silicon metasurface also acts as a homogeneous core layer that support slab waveguide modes, governed by TIR [224]. **Figure 4-1(c)** shows the dispersion of a thin film slab waveguide, where the light line is defined by the dispersion relation $|k| = n \frac{\omega}{c}$, which relates the wavevector (k), frequency (ω), speed of light in vacuum (c), and refractive index of waveguide material (n). The modes that lie above the light line are radiative in nature, while those lying below are guided within the slab waveguide. In the case of patterned silicon layer, the waveguiding criteria of the effective slab waveguide can be expressed as $k = \frac{\omega}{c} n_g \sin(\theta)$, where n_g is the average refractive index of the effective slab waveguide and θ is the angle of incidence at the interface of slab waveguide and top cladding (refractive index of n_c). Since, the slab waveguide is a periodic structure, it leads to the translation symmetry of the band structure in the reciprocal space. In a first approximation, the band structure is a repeated band of homogeneous layer, as shown in **Figure 4-1(c)** being enumerated as -1, 0, +1 and so on. Due to band folding, the guided modes now fall above the light line and hence become guided resonances that couple to the radiating modes of the cladding. The combination of the waveguiding criteria (i.e. TIR) and the grating equation provides the critical condition for the realization of GMR, which is given by: $n_c < \sin(\theta) - m \frac{\lambda}{\Lambda} < n_g$ [199, 224], where Λ is the lattice period, λ is wavelength and frequency is given by $f = c/\lambda$. By solving the GMR equation, a pair of GMRs can be readily achieved as a function of θ . In the vicinity of Γ point ($\theta = 0^\circ$), rigorous calculations account for the interaction of these resonance modes, which show either anti-crossing behavior indicating a strong coupling regime [173, 228], or cross-

over behavior implying a weak coupling regime [173, 229], as highlighted by the blue and red dispersion curves in **Figure 4-1(e)**, respectively. Earlier works in PhC membranes show anti-crossing behavior due to the periodically modulated dielectric function, which introduces a gap opening and flattening of the dispersion at the center of the Brillouin zone [45, 229]. The 180° rotational symmetry (C_2) of these structures ensures the modes at the Γ point to be either odd or even. The mode splitting at the Γ point results in existence of pure odd modes, which are decoupled from the propagating modes in the cladding due to the symmetry, and results in a symmetry-protected BIC [77]. However, these interactions in the weak coupling regime (**Figure 4-1(e)** red curve) for excitation of BIC is not very well understood. Our metasurface that supports GMRs also provides a platform for the detailed investigation of BIC excitation in the weak coupling regime.

The numerical simulations were carried out using CST microwave studio solver for the angle-resolved transmission spectra of the metasurfaces. The simulated results for silicon cuboid resonators with $L = 270 \mu\text{m}$, $W = 180 \mu\text{m}$ at varying θ are shown in **Figure 4-2(a)**, and $L = 270 \mu\text{m}$, $W = 210 \mu\text{m}$ are shown in **Figure 4-2(b)**, respectively. Periodic boundary conditions were applied in both x - and y -directions and TM (E_x, H_y, H_z) polarized wave was employed to excite the metasurface. Both metasurfaces show counter propagating mode splitting as function of the angle of incidence, as shown in **Figures 4-2(a)** and **4-2(b)**, which implies the observation of GMRs. To fabricate the samples, $1.5 \mu\text{m}$ -thick SiO_2 was first deposited onto $200 \mu\text{m}$ -thick silicon wafers. Later, photoresist with thickness of $2 \mu\text{m}$ was spin coated and conventional photolithography created metasurface patterns on the photoresist. After developing the patterns, the SiO_2 coated silicon wafers with photoresist structures were stuck to a 1 mm -thick quartz ($n_{\text{Quartz}} = 2.14$) substrate using UV glue (NOA 85-Norland Products, Inc., $n_{\text{glue}} = 1.48$). RIE was used to pattern the $1.5 \mu\text{m}$ -thick SiO_2 layer which acts as a hard mask for the silicon etching (details in chapter 3). Finally, the deep RIE was carried out to etch silicon to obtain the

desired samples. The SEM images of fabricated sample are shown in **Figures 4-1(a) and 4-1(b)**.

Figure 4-2. Numerical simulations and experimental measurements of the GMRs in all-dielectric terahertz metasurface. (a), (b) Angle-resolved transmission spectra. The top panel (a) corresponds to the silicon cuboid resonator with geometric parameters of $L = 270 \mu\text{m}$, $W = 180 \mu\text{m}$, and the bottom panel (b) corresponds to the silicon cuboid resonator with geometric parameters of $L = 270 \mu\text{m}$, $W = 210 \mu\text{m}$, respectively. (c), (d) Experimentally measured transmission spectra at different incidence angles from 6.84° (bottom) to 21.84° (top) for the metasurfaces with $W = 180 \mu\text{m}$ (c) and $210 \mu\text{m}$ (d), respectively. (e), (f) Corresponding measured transmission spectra as function of angle of incidence for the metasurfaces with $W = 180 \mu\text{m}$ and $210 \mu\text{m}$, respectively. The inset figures are the numerically simulated real part of electric field E_z component for +1 and -1 order GMRs at 6.84° , respectively.

The transmission spectra of the all-dielectric metasurfaces were performed using a fiber-based THz-TDS system. In order to enable experimental observation of high- Q resonances, the time-domain scan should be large enough to provide spectral resolution on the order of the resonance

linewidths. Long scan measurements with terahertz pulses can be challenging due to the etalon pulse from the substrate. To delay the etalon pulse, we stuck the fabricated samples to a thick quartz (thickness of 10 mm) substrate with an ideal optical contact. This allowed for the maximum scan length of ~ 157 ps, which corresponds to a frequency resolution of 6.37 GHz and the maximum measurable Q -factor of 62.79 at 0.4 THz. Further, the emitted time-domain terahertz beam was focused to a spot size of 10 mm in diameter by a lens with aperture diameter of 22 mm and focal length of 50 mm. Focusing of terahertz beam limits the minimum achievable θ of 6.84° . For THz-TDS, the transmitted time-domain signals through the samples were transformed to frequency domain and normalized by the transmission signal through an identical bare quartz substrate as the reference. Therefore, the transmission is given by $|\tilde{T}(\omega)| = |\tilde{E}_s(\omega)/\tilde{E}_R(\omega)|$, where $\tilde{E}_s(\omega)$ and $\tilde{E}_R(\omega)$ are the Fourier transformed transmission spectra for the sample and the reference, respectively.

As shown in **Figures 4-2(c) and 4-2(d)**, the angle-resolved transmission spectra for $W = 180$ μm and 210 μm were measured by rotating the samples with central angles (Φ) of $0^\circ, \pm 5^\circ, \pm 10^\circ$, and $\pm 15^\circ$. This corresponds to the angles of incidence (θ) of $6.84^\circ, \pm 11.84^\circ, \pm 16.84^\circ$, and $\pm 21.84^\circ$, respectively. Therefore, the normal incidence is absent, and the measured spectra always show non-degenerate GMRs, with the +1-order GMR at lower frequency and -1-order GMR at higher frequency. Due to the C_2 rotational symmetry of the metasurface, the ± 1 -order GMRs show almost same resonant frequency for the positive and negative θ . It is clearly observed that the mismatch (resonance amplitude and frequency) of ± 1 -order GMRs becomes obvious as Φ reaches $\pm 15^\circ$. The transmission measurements were restricted to the maximum θ of $\pm 21.84^\circ$ ($|\theta| \leq 21.84^\circ$) as the THz beam gets misaligned from the sample at larger angles due to the presence of thick (11 mm) quartz substrate.

To compare the numerical simulations and experimental measurements with the GMR theory, we extracted GMR trajectories (transmission minima) for the simulated data as shown in **Figures 4-2(a) and 4-2(b)** and experimental data plotted in **Figures 4-2(c) and 4-2(d)**, respectively. Spectral minima of the ± 1 -order GMRs are plotted in **Figure 4-2(e)** for $W = 180 \mu\text{m}$ and in **Figure 4-2(f)** for $W = 210 \mu\text{m}$, where the gray region shows the theoretically calculated GMRs from $n_c < \sin(\theta) - m \frac{\lambda}{\Lambda} < n_g$. Experiments show good agreement with the theoretical calculations and numerical simulations. Some minor deviations are observed, which could originate due to the lower refractive index of the UV glue ($n = 1.48$) that was used to bond the silicon resonators on quartz substrate. The limited resolution ($\sim 6.37 \text{ GHz}$) of our THz-TDS system also restricts the maximum value of measured resonance amplitude. In addition, the presence of diffraction mode at 0.47 THz also results in the non-normal diffractions and the suppression of the normal transmission, which is the main reason for large discrepancy between theory and simulation for -1-order GMR above this frequency, as shown in **Figure 4-2(e) and Figure 4-2(f)**. To elucidate the characteristics of GMRs in our metasurface, the electric field (real part of E_z component) was simulated at the resonance frequencies as shown in the inset of **Figure 4-2(e) and 4-2(f)**. For $\theta = 6.84^\circ$, the +1-order GMR propagates in $-x$ direction while the -1-order GMR propagates in the $+x$ direction, respectively.

Moreover, the metasurface with $W = 210 \mu\text{m}$ shows an additional resonance around 0.457 THz , which is independent of θ , as shown in **Figure 4-2(b) and Figure 4-2(d)**. This additional resonance corresponds to the flat-band of photonic band structure that stems from the nearest-neighbor coupling of the silicon cuboid resonators [45, 230]. In the metasurface, the silicon cuboid resonators are periodically arranged in x - O - y plane, which implies that the magnetic field along y -axis is periodically modulated. The magnetic field remains parallel to the horizontal plane (x - O - y plane) such that the magnetic coupling between silicon resonators remains constant without dependence on θ . Hence, the resonance induced due to magnetic

coupling remains unchanged as θ increases. This resonance mode is not observed in the metasurface with $W = 180 \mu\text{m}$, owing to the reduced coupling between the nearest neighbors.

4.4 Additional measurements

To further verify the observation of GMRs, we numerically simulated and experimentally measured two additional samples with the geometric length of $260 \mu\text{m}$, and width of $210 \mu\text{m}$ and $180 \mu\text{m}$. Similar to the previous case, the GMRs are degenerated under normal incidence and split into two counter propagating modes that correspond to the +1-order and -1-order GMRs once the incident wave is tilted, as shown in **Figure 4-3**. The experimentally measured transmissions are also plotted in **Figures 4-3(a)** and **4-3(b)**, where excellent agreement between the measurement and simulation is demonstrated. Similar to the previous case, the GMRs are degenerated under normal incidence and split into two counterpropagating waves that correspond to the +1-order and -1-order GMRs once the incident wave is tilted.

Figure 4-3. Additional experiments. (a) The sample under measuring has geometric parameters of $L=260 \mu\text{m}$, $W=180 \mu\text{m}$, while (b) corresponds to the device with geometric parameters of $L=260 \mu\text{m}$, $W=210 \mu\text{m}$.

4.5 Localized field enhanced by symmetry-protected bound states in the continuum

We further analyze the interactions between degenerate modes near the Γ point by finely varying the angle of incidence ($-5^\circ \leq \theta \leq 5^\circ$). **Figures 4-4(a)** and **Figures 4-4(b)** show the simulated transmission spectra at small angles of incidence for the metasurface with $W = 180 \mu\text{m}$ and $210 \mu\text{m}$, respectively. As θ decreases from 5° , the two GMRs for the metasurfaces come close to each other and finally push the transparency peak to the symmetry-protected BIC mode. For metasurface with $W = 180 \mu\text{m}$, two GMR dips show a “Dirac”-like crossing behavior, indicating that the degenerate modes are in the weak coupling regime (same to **Figure 4-1(e)** the red curve). show the simulated transmission spectra at small angles of incidence for the metasurface with $W = 180 \mu\text{m}$ and $210 \mu\text{m}$, respectively. As θ decreases from 5° , the two GMRs for the metasurfaces come close to each other and finally push the transparency peak to the symmetry-protected BIC mode. For metasurface with $W = 180 \mu\text{m}$, two GMR dips show a “Dirac”-like crossing behavior, indicating that the degenerate modes are in the weak coupling regime [45, 229]. Therefore, two GMRs form an anti-crossing behavior at normal incidence that verifies the strong (enhanced magnetic) coupling (same as **Figure 4-1(e)** blue curve).

To further analyze the symmetry-protected BICs, we also calculated the Q -factor and average field enhancement $\langle E \rangle / |E_0|$ for both metasurfaces, where E_0 is the incident field amplitude and $\langle E \rangle = \frac{1}{V} \int |\mathbf{E}(\mathbf{r})| d\mathbf{r}$ is the averaged electric field over the resonator volume, $\mathbf{E}(\mathbf{r})$ is the field distribution in 3D coordinates $\mathbf{r} = (x, y, z)$. **Figure 4-4(c)** shows that the confined field intensity at the transmission peaks, which is fitted by $I = I_0 |\sin\theta|^{-2}$, where $I = \langle E \rangle^2 / E_0^2$. **Figures 4-4(c)** shows the calculated Q -factors of the transmission peaks, which is fitted by $Q = Q_0 |\sin\theta|^{-2}$. Note that both the field enhancement and Q -factor has the α^{-2} dependence (α is the asymmetry parameter and $\alpha = |\sin\theta|$), which diverges to ∞ at $\theta = 0^\circ$, thereby revealing the symmetry-protected nature of BIC [231]. Hence, GMR is inherently a symmetry-protected BIC system at normal incidence and the trapped modes become leaky, i.e. finite Q -

factor, and the enhancement of field localization reduces as the angle of incidences goes off-normal.

Figure 4-4. Numerical simulations of the terahertz GMRs near the Γ point. (a), (b) Calculated transmission spectra for the silicon cuboid with $W = 180 \mu\text{m}$ and $W = 210 \mu\text{m}$, respectively for angle of incidence from -5° to 5° . (c) Corresponding enhancement of averaged intensity ($\langle E \rangle^2$) inside the silicon cuboid at the transmission peak for small angles of incidence. (d) The calculated Q -factors of the transmission peaks in (a) and (b).

4.6 Parameter optimization

Furthermore, geometrical parameters of the silicon cuboid resonators play a crucial role in the design of GMRs. Here, the effect of resonator length L on the GMRs was studied by varying L from $180 \mu\text{m}$ to $300 \mu\text{m}$, while keeping the width constant at $210 \mu\text{m}$. **Figures 4-5(a)** and

Figures 4-5(b) show the simulated transmission spectra of the metasurface with varying length for $\theta = 0^\circ$ and 6.84° , respectively. At normal incidence, a single GMR was observed at 0.45 THz for $L = 180 \mu\text{m}$. With increasing L , a continuous redshift of the single GMR was observed, which is due to the increased mode volume of the resonator cavity. For $L = 300 \mu\text{m}$, the degenerated GMRs shift to lower frequency of 0.375 THz. However, for the case of $\theta = 6.84^\circ$, a clear mode splitting was observed around the degenerate GMR frequency for all lengths.

Figures 4-5(c) shows the experimentally measured transmission spectra for the metasurface with increasing L . For L less than $240 \mu\text{m}$, higher frequency branch (-1 order) of the GMR is suppressed due to the interference of the higher order Rayleigh diffraction mode in the system.

Figure 4-5. Simulated and measured transmission spectra for terahertz GMRs in metasurfaces with increasing resonator length (L). (a), (b) Simulated transmission spectra of the metasurface

with varying silicon cuboid resonator length L for the angle of incidence of 0° (top panel) and 6.84° (bottom panel), respectively. The dashed black line indicates the first-order Rayleigh diffraction mode at 0.468 THz. (c) Measured transmission spectra of the metasurface device at angle of incidence $\theta = 6.84^\circ$ by changing length of the silicon cuboid resonator L from 220 μm to 280 μm with a step size of 10 μm .

It is important to note that these Rayleigh diffractions also shift to low frequency accordingly with increasing angle of incidence. Therefore, an ideal design to achieve clear GMRs at large angle of incidence is to increase the geometric length of the silicon cuboid, as shown in the transmission spectra for L larger than 240 μm in **Figures 4-5(b)**. The measured transmission spectra in **Figures 4-5(c)** show similar trends as the numerically simulated transmission spectra in **Figures 4-5(b)** even though the diffraction boundaries are not well resolved. However, the ± 1 -order GMRs for $L > 240 \mu\text{m}$ appear clearly in the transmission spectra, which match well with the numerical simulations.

4.7 Conclusion

In this chapter, we have experimentally demonstrated terahertz guided mode resonances in all-dielectric metasurface consisting of a 2D array of silicon cuboid resonators. The metasurface shows two counterpropagating GMRs at oblique incidence, and the spectral difference between their resonance frequencies increases with increasing angle of incidence. However, at very small angles of incidence ($0^\circ < |\theta| \leq 1^\circ$), the destructive interference between the counter propagating GMRs (± 1 -order modes) enable extremely high- Q resonances that eventually leads to *symmetry-protected BICs* with infinite Q -factor at normal incidence. Our results present an experimental observation of THz GMRs in 2D all-dielectric metasurfaces. This opens up a new route for realizing efficient on-chip THz communication components, such as

wavelength selective polarizer, beam splitters, differentiators, integrators, and wavelength division multiplexers.

Chapter 5: In-plane symmetry breaking induced terahertz bound states in the continuum

5.1 Introduction

Enhancement of wave localization in PhC slabs and metasurfaces has led to the experimental investigations of novel physics phenomena in both fundamental and applied research [77, 165, 166, 170, 173]. This is typically achieved by engineering high- Q factor cavities, where the wave is trapped for a longer period before leaking out [77]. Hence, high- Q cavities are critical for applications enabled through light-matter interactions, such as low-threshold lasing [97, 232], high-order harmonic generation [94, 95, 179, 180, 181, 203-206], and ultrasensitive bio-/chemical sensing [98-100]. There has been a mass of relentless quests for realizing an ideal cavity which can trap light wave for infinite time τ . Recently, optical bound states in the continuum (BIC) seems to be promising route for achieving infinite- Q cavities, where the trapping mode in a non-radiating state coexist within the continuous spectrum of radiating waves [77, 94, 165, 166, 98-100]. Initially, the BIC concept was predicted by von Neumann and Wigner in quantum mechanics [58]. Due to the universal nature of waves, the existence of BICs has also been widely investigated in various fields, such as quantum mechanics, water waves, acoustic waves, mathematics, and electromagnetic waves ranging from microwave to optical regime [77], et al.

PhC slabs and metasurfaces are widely used platforms for the experimental investigation of BICs due to their arbitrary building block and size-dependent frequency tunability [77-80, 94, 165, 166, 98-100]. The BIC modes in the PhC slabs and metasurfaces are usually categorized as [77, 81]: symmetry-protected BICs, which exists at the Γ point, where the coupling to the free space is forbidden due to symmetry mismatch between planewave and PhCs, and off- Γ BICs, which are unprotected by symmetry and can occur at unpredicted angle of incidence. All BICs are topologically protected by vortex centers in the polarization of far-field radiation that

is fundamental to optical BICs [90]. However, the BICs at normal incidence are better suited for real-world applications since the normal direction is more convenient, feasible, and compact than the oblique ones [98-100, 233, 234]. Therefore, the important question is how the structural symmetry plays significant role in tailoring accessible BICs. A trivial version of symmetry breaking is to use oblique incidence that breaks the even in-plane symmetry of the incident planewave [77, 81, 82, 90, 232]. Alternatively, the symmetry can be reduced by breaking rotational or mirror symmetries of the structural elements [232-234]. Compared to the symmetry breaking of plane wave under angular incidence, the structural symmetry breaking provides additional degrees of freedom for device building block and applying BICs to the real-world applications. Therefore, it has become one of the most active research fields in realizing BIC [203-206, 232-234]. In 2018, Nguyen et al. reported that the breaking of the vertical mirror symmetry in dielectric PhCs allows for the dispersion engineering of the PhCs to be Dirac cone, flat band, or parabola [233]. Later, Wang et al applied the same principle to bilayer honeycomb PhC slab for both TE and TM symmetry-protected BICs as well as the enhancement of TE-TM polarization coupling due to broken mirror-flip symmetry [234]. Koshelev et al summarized a universal law for in-plane symmetry breaking in metasurfaces and PhC slabs, where the mode linewidth is purely controlled by the degree of asymmetry [231].

In this chapter, we report a new class of in-plane symmetry-broken subwavelength cross-type silicon metasurfaces to excite BICs in terahertz regime. The concept of metasurface is employed due to their highly compact building block at the subwavelength scales. Above the light cone, the metasurfaces with the in-plane C_{4v} symmetry supports a flat band as the TM_1 and a W-shape band as the TM_2 , both support symmetry-protected BICs at the Γ point. It also shows off- Γ BICs for the TM_2 band. Then, the in-plane rotational symmetry can be lifted by displacing the vertical dielectric bar (that is a part of the cross) along the x-axis (d_x). We therefore observe additional BICs apart from the symmetry-protected one. The mechanism of

such BICs is interpreted as the destructive interference of different propagating Fourier wave components. Finally, we measure these BICs at the quasi-states to confirm the existence of such symmetry-broken BICs at terahertz regime.

5.2 Bound states in the continuum in C_{4v} photonic lattice

To reveal the excitation of BICs in dielectric metasurface under symmetry consideration, we start with a square lattice ($\Lambda = 150 \text{ } \mu\text{m}$) of symmetric dielectric crosses, as shown in **Figure 5-1(a)**. Each dielectric cross has length (L) of $130 \text{ } \mu\text{m}$ and width (W) of $40 \text{ } \mu\text{m}$. The metasurfaces are made up of high resistivity silicon with thickness (H) of $100 \text{ } \mu\text{m}$ and refractive index of 3.48 in the spectral region of interest. Here, the cladding layers of superstrate and substrate are set as air to preserve the mirror symmetry in the z -axis. Therefore, the structure is invariant under symmetry operations from the C_{4v} point group. For a two-dimensional lattice, six types of eigenmodes, i.e. two doubly-degenerate modes $E^{(1)}$ and $E^{(2)}$, and four non-degenerate modes $A_{1,2}$ and $B_{1,2}$ can be classified according to their lateral symmetries [45, 235, 236].

The calculated band structure of the C_{4v} lattice is shown in **Figure 5-1(b)**, where we focus on the two lowest TM-like bands (referred to as TM_1 : black, and TM_2 : cyan). By closely studying the band structure in a larger scale and angle-resolved transmission map, it is observed that the TM_1 band shows a flat dispersion and TM_2 band demonstrates a W-shaped dispersion, as shown **Figure 5-1(b)**. The Q -factors of TM_1 and TM_2 bands in the k -space are shown in **Figures 5-1(c)** and **5-1(f)**. The TM_1 band exhibits one BIC at the center of Brillion zone (Γ point), as shown in **Figures 5-1(c)** and **5-1(d)**. However, the TM_2 band supports four additional BICs at the certain wavevector (k_x, k_y) away from the Γ point, as shown in **Figures 5-1(f)** and **5-1(g)**. Theoretical and experimental investigations have verified both symmetry-protected and additional BICs are topologically protected by polarization vertices [90]. As for the four additional BICs, they have identical topological charges that are opposite to the one at the Γ point [36]. The topological properties of the BICs are also understood by fitting the Q -factors

as function of the in-plane wavevectors, as shown in **Figures 5-1(d)** and **5-1(g)**. For both TM_1 and TM_2 bands, their Q -factors show quadratic decay ($Q \propto 1/k^2$) with respect to the in-plane wavevectors. Specifically, Q -factor of the TM_1 band shows $Q \propto 1/k^2$ and it is $Q \propto 1/k^2 + 1/(k - k_{BIC})^2 + 1/(k + k_{BIC})^2$ for the TM_2 band. It is therefore demonstrated that all BICs are isolated [237]. We also notice that the Q -factor is ill-fitted at the two concaves due to the strong coupling between TM_1 and TM_2 bands. As shown in **Figure 5-1(b)**, the anti-crossing behavior of these two bands also confirms the exchange of energy between them due to strong coupling.

Figure 5-1. Theoretical predictions of C_{4v} rotationally symmetric dielectric metasurface. (a) Schematic view of the metasurface with silicon building block. The unit cell is plotted by the C_{4v} rotational symmetry and the axes of mirror symmetry are labeled as σ_x , σ_y , σ'_d and σ''_d . The corresponding first Brillouin zone is plotted at the bottom of unit cell. (b) Numerically simulated band structure. The bands under consideration are above the light cone (dashed black line). The TM_1 band demonstrates flat band and symmetry-protected BICs, and the TM_2 band shows both symmetry-protected as well as off- Γ BICs. The inset transmission map is zoomed for visualization of flat band (TM_1) and W-shape (TM_2) band. (c) The radiating Q -factors of the TM_1 band plotted in the k -space, and (d) $Q \propto 1/k^2$. (e) The corresponding mode profile (E_z) on $z = 0$ plane shows B_1 irreducible representation for the symmetry-protected BIC on TM_1 band. (f) The radiating Q -factor of TM_2 band shows symmetry-protected BIC at Γ point and off- Γ (“accidental”) BICs at the unexpected wavevector k , and (g) $Q \propto 1/k^2 + 1/(k - k_{BIC})^2 + 1/(k + k_{BIC})^2$. (h), (i) The mode profiles at the symmetry-protected and accidental BICs given by real parts of E_z show A_1 and A irreducible presentations according to the group theory.

To further understand both symmetry-protected and additional BICs, we analyze the symmetry properties of the mode profile (real parts of E_z) at the BIC state. The mode profile of the symmetry-protected BIC on TM_1 band at the Γ point is shown in **Figure 5-1(e)**. The symmetry operations $\{E, C_4, C_4^{-1}, C_2, \sigma_x, \sigma_y, \sigma'_d, \sigma''_d\}$ are given by the characters $\{1, -1, -1, 1, 1, 1, -1, -1\}$, where the symmetric overlapping after operation is given by 1 and the antisymmetric overlapping after operation is -1. Therefore, the symmetry-protected BIC on TM_1 band at the Γ point demonstrates itself as a B_1 irreducible representation of the C_{4v} point group [45, 236]. Figure 1(h) shows the mode profile of the symmetry-protected BIC on TM_2 band at the Γ point, where the symmetry operations $\{E, C_4, C_4^{-1}, C_2, \sigma_x, \sigma_y, \sigma'_d, \sigma''_d\}$ equal to $\{1, 1, 1, 1, 1, 1, 1, 1\}$.

Therefore, the TM_2 band at the Γ point belongs to the A_1 irreducible representation of the C_{4v} point group. Moreover, it can also be observed that the accidental BICs for TM_2 band at Δ point in the Brillion zone, i.e. unpredicted (k_x, k_y) , that belongs to the A irreducible representation of a C_{1h} point group according to the compatibility relations [45]. By classifying the irreducible presentations (non-degenerated A_I, B_I) of the bands under investigation, it is easy to prove that they decouple from the radiation continuum due to their orthogonality to the plane waves with x - and y -polarizations [235]. Therefore, symmetry-protected BICs are due to the absence of the coupling of the non-degenerated A_I and B_I modes to outside radiation at the Γ point on the TM_1 and TM_2 bands. As for the accidental BICs on TM_2 band, they are interpreted as the destructive interference between various leakage channels [83].

5.3 In-plane C_{4v} symmetry breaking

We first focus on the scenario that the vertical silicon bar is horizontally displaced away from the center by distance of d_x along the x -axis, as shown in **Figure 5-2(a)**. This leads to the breaking of the C_4 rotational symmetry but preserves the mirror symmetries σ_y , thereby reducing the point group to be C_{1h} . This does not allow symmetry protected BIC since its both representations are coupled to a plane wave. The transmission map is plotted in **Figure 5-2(b)** as function of d_x and frequency, where $t(d_x, \bar{\omega})$ is the transmission amplitude, and $T = |t|^2$ is the transmittance under TM polarized (E_x, H_x, H_z) excitation. Without symmetry breaking, i.e. $d_x = d_y = 0 \mu m$, the symmetry-protected BICs are observed for both TM_1 and TM_2 bands, as shown in **Figure 5-1**. In addition, only the symmetry-protected BIC is observed for the TM_1 band so that the Q -factor continuously decreases with the displacement d_x . However, for the TM_2 band, two additional BICs are observed at $d_x = 15.3 \mu m$ and $d_x = 38 \mu m$, where the symmetry is broken, as shown in **Figure 5-2(c)**. These two BICs violate the inverse-square law dependence on the asymmetry parameter for the symmetry-protected BICs [231], thereby drawing intense interests. Usually, the BICs transform into quasi-states if the in-plane

symmetry gets broken. However, the new BIC states are excited due to the destructive interference of leaky channels at the slab-medium interfaces. The field profile in Fourier expansion existed inside the dielectric slab layer can be expressed as a superposition of waves with different propagation constants β_z in z direction. Each wave from different β_z channels at the slab-medium interface destructively interfere with each other, leading to the complete disappearance of leakage [82, 146]. Quantitatively, this argument is verified by varying the dielectric slab thickness, as shown in **Figures 5-2(d) and 5-2(e)** for $d_x = 15.3 \mu m$ and $d_x = 38 \mu m$, respectively. The transmission map as function of normalized slab thickness and normalized wavelength is calculated with the RCWA algorithm, where only the propagating Fourier components (real β_z in z direction) is calculated, as shown in **Figures 5-2(d) and 5-2(e)**. The transmission maps show three regions: the diffraction region at short wavelength, the Fabry–Pérot fringes at longer wavelength, and an interference region between them [50]. We therefore observed the BIC features at $H = 100 \mu m$ for the TM_2 band, as labeled by the blue line in **Figures 5-2(d) and 5-2(e)**. Moreover, both TM_1 and TM_2 modes (and their higher order modes) can be non-radiating BICs (blue circles) at the same time by fine tuning the thickness of the metasurface slab.

We also calculated the spatially averaged field enhancement, given by $E_{avg} = \frac{1}{V} \int_V |E(\mathbf{r})| dv$ where V is the volume of the unit cell, $\mathbf{r}$ is the 3D coordinate, both inside and outside the dielectric structure for the TM_1 and TM_2 modes, as shown in **Figure 5-2(f)**. It shows that the sample with displacement of d_x has large field enhancements (normalized to field at the incident plane E_0) for both inside (solid curves) and outside (dashed curves) of the silicon crosses. Moreover, the field enhancements diverge to infinity at the BIC conditions. The inside field enhancements are slightly larger than the outside ones while they share same trends as a function of displacements d_x .

Figure 5-2. In-plane symmetry breaking the dielectric metasurfaces by displacing the vertical silicon bar. (b) Transmission map as function of the frequency and displacement d_x . (c) The corresponding Q -factors of the TM_1 and TM_2 bands as function of d_x . (d), (e) The numerically calculated transmission maps as function of the slab thickness H for $d_x = 15.3 \mu m$ and $d_x = 38 \mu m$, respectively. (f) The field enhancements inside and outside of the devices as function of d_x .

The horizontal silicon bar can also be vertically displaced away from the center by distance of d_y along the y -axis that breaks the C_2 rotational symmetry but preserves mirror symmetries σ_x . This operation allows the TM_3 mode to be excited. It is clearly observed that only a symmetry-protected BIC is observed for $d_y = 0 \mu m$, as shown in **Figure 5-3(a)** by the transmission map as function of d_y . The Q -factor decreases monotonously as the displacement increases such that the inverse-square law is valid [231]. Therefore, we omit the quantitative analysis on this mode. Finally, both vertical and horizontal silicon bars are displaced from center by distances of d_x and d_y , where no symmetry is found for such operation if $d_x \neq d_y$, except the trivial symmetry.

However, the C_{1h} point group is preserved for $d_x = d_y$, in which all three modes (TM₁, TM₂ and TM₃) are excited. The transmission spectra as a function of $d_x = d_y$ are plotted in **Figure 5-3(c)**. The TM₃ mode supports only symmetry-protected BIC at highest frequency such that the analysis on it is skipped. However, the TM₁ and TM₂ modes show additional BICs, at $d_y = 15 \mu\text{m}$ for the TM₁ and $d_x = d_y = 24 \mu\text{m}$ for the TM₂, respectively. With extended BICs excited, the Q -factor trends to infinite, as shown in **Figures 5-3 (b)** and **5-3 (d)**.

Figure 5-3. Two additional methods show in-plane symmetry breaking of the dielectric metasurfaces. (a) The numerically calculated transmission spectra, and (b) Q -factors of the devices as function of d_y with $d_x = 0$. (c) The numerically calculated transmission spectra, and (d) Q -factors of the devices as function of d_x and d_y with $d_x = d_y$.

5.4 Fabrication and measurement

The samples were fabricated by using high-resistivity silicon ($>10000 \text{ } \Omega \cdot \text{cm}$) due to its low loss and dispersionless characteristic ($n_{\text{Si}} = 3.48$) at terahertz frequencies. To fabricate the samples, SiO_2 film with thickness of $1.5 \text{ } \mu\text{m}$ was first deposited onto silicon wafers with thickness of $100 \text{ } \mu\text{m}$. Then, photoresists with thickness of $2 \text{ } \mu\text{m}$ were spin-coated, and standard mask photolithography was employed to create the desired patterns on the photoresist. After developing, the SiO_2 /silicon wafers with photoresist patterns were stacked onto a quartz ($n_{\text{Quartz}} = 2.14$) substrate with thickness of 1 mm by employing UV glue (NOA 85-Norland Products, Inc., $n_{\text{glue}} = 1.48$) with thickness of $80 \text{ } \mu\text{m}$. The RIE process was utilized to pattern metasurface structure on the SiO_2 layer with thickness of $1.5 \text{ } \mu\text{m}$ which plays a mask role for next step. Finally, the DRIE process was employed to etch the silicon film to obtain the designed samples. The fabricated sample images are captured by the SEM, as shown in **Figure 5-3(a)**. Each bar element of the dielectric cross resonator has a length of $L = 130 \text{ } \mu\text{m}$, width of $W = 40 \text{ } \mu\text{m}$, and height of $H = 100 \text{ } \mu\text{m}$. The normalized transmission of the all-dielectric metasurfaces were achieved by using a fiber-based THz-TDS setup (T-Ray® 5000), which is employed for generation of terahertz radiation and detection, as shown in **Figure 5-3(d)**. To delay an undesired echo signal and capture a longer terahertz scan length, the samples ($100 \text{ } \mu\text{m}$ -thick silicon metasurface on quartz substrate with thickness of 1 mm) were staked onto an identical quartz substrate with thickness of 10 mm . Therefore, the first echo was delayed by $\sim 157 \text{ ps}$ such that the frequency-domain spectrum shows resolution around $\sim 6.37 \text{ GHz}$ that is applicable for experimental resonance with Q -factor around ~ 150 at 0.95 THz . Finally, the emitted time-domain terahertz signal is focused onto a spot in diameter of 10 mm by a lens with diameter of 22 mm and focal length of 50 mm , which leads to the convergence angle $\theta = 6.84^\circ$ of the incidence terahertz beam. For THz-TDS, the captured time-domain signals were transformed to the frequency domain and normalized by using the identical bare quartz

substrate as a reference. The normalized transmission spectrum in frequency domain is $|\tilde{T}(\omega)| = |\tilde{E}_S(\omega)/\tilde{E}_R(\omega)|$, where $\tilde{E}_S(\omega)$ and $\tilde{E}_R(\omega)$ are the spectra of sample and reference after Fourier transform, respectively.

Figure 5-4. Fabricated samples and fiber-based THz-TDs measurement. (a) The top view of fabricated sample with C_{4v} symmetric silicon cross sitting in a periodic lattice $\Lambda = 150 \mu\text{m}$ and (b) the perspective view of the C_{4v} symmetric silicon cross with length $L = 130 \mu\text{m}$, width $W = 40 \mu\text{m}$, and thickness $t = 100 \mu\text{m}$. (c) The top view of fabricated sample with in-plane symmetry broken by horizontally shift the vertical dielectric bar from the center with displacement of $d_x = 30 \mu\text{m}$. The images were taken by scanning electron microscope (SEM). (d) The schematic view of fiber-based THz-TDS measurement setup. The emitted terahertz pulse is focused by a lens with focal length of $f = 50 \text{ mm}$, and diameter of 22 mm, and then it passes through the sample with total area of 10 mm by 10 mm and is detected at the terahertz receiver.

5.5 Experimental observation of terahertz quasi-BICs

To experimentally measure the quasi-BICs of in-plane symmetry broken in our metasurface, four samples with the x -axis displacement d_x of 0 μm , 10 μm , 30 μm , and 40 μm were

fabricated and measured. **Figure 5-5(a)** shows the experimentally (red) measured and numerically (black) calculated transmission spectra. The experimental data match well with that of theory. Since the fiber-based THz-TDS contains focal lens such that the terahertz pulse is converged at an angle of incidence $\theta = 6.84^\circ$, two quasi-BICs are observed even when the displacement d_x is zero. To clearly demonstrate the transmission evolution as a function of d_x , the transmission maps are plotted in **Figures 5-5(b)** for $\theta = 6.84^\circ$ and **5-5(c)** for $\theta = 0^\circ$, respectively. Here, the quartz substrate and the UV glue as a middle layer are taken into consideration for matching the experiments (as discussed before, $n_{glue} = 1.48$ and $t_{glue} = 80\mu m$). By considering 6.84° as the incident angle, as shown in **Figure 5-5(b)**, the two quasi-BICs are always observed no matter how the x -axis displacement d_x changes. It should be noticed that the TM_1 and TM_2 modes cross each other as $d_x > 20\mu m$, as shown in **Figures 5-4(d) to 5-4(k)**. However, the symmetry-protected BICs as well as the symmetry-breaking BICs can be resolved once the terahertz wave impinges on the sample at normal incidence, as shown in **Figure 5-4(c)**. We also observed that the peak field enhancement is more than 20 times even through the BICs are experimentally measured at the quasi-states, as shown in **Figures 5-5(d) to 5-5(k)**.

Figure 5-5. Experimentally measured quasi-BICs by varying the x -axis displacements d_x . (a) Comparison between the measured (red) and calculated (black) transmission spectra at different x -axis displacements d_x . Evolution of the calculated transmission map vs. x -axis displacement d_x and frequency (b) angle of incidence $\theta = 6.84^\circ$ and (c) normal incidence $\theta = 0^\circ$. (d)-(k) mode profiles (real parts of E_z) of the transmission channels (blue stars in (a) and (b)) that correspond to the perturbed B_1 and A_1 irreducible representations. The angle of incidence is 6.84° and the mode profiles show enhancement more than 20 times.

Figure 5-6. Experimental measurements of the quasi-BICs by varying the y -axis displacements d_y . (a) Comparison between the measured (in deep colors) and calculated (in undertint colors) transmission spectra at different y -axis displacements d_y . Evolution of the calculated transmission map versus frequency and y -axis displacement d_y (b) angle of incidence $\theta = 6.84^\circ$ and (c) normal incidence $\theta = 0^\circ$.

By rotating the sample by 90° , we have samples with y -axis displacements d_y , as shown in **Figure 5-6(a)**. Similar to the x -axis displacement, the transmission spectra also show two stable quasi-BICs as d_y increased under incident angle of 6.84° , as shown in **Figure 5-6(a)** and **5-6(b)**. However, only a single symmetry-protected BIC is observed at $d_y = 0 \mu m$ for the normal incidence. In **Figure 5-6**, the UV glue and quartz substrate are both taken into consideration, which implies the breaking of vertical mirror symmetry. As also discussed in **Figure 5-3**, the duration of the scan length (time-main pulse) limits the frequency resolution around ~ 6.37 GHz such that the real-BICs and quasi-BICs with Q -factor larger than 150 (around 1 THz) are undetectable. Therefore, high-resolution and angular-resolved terahertz spectroscopy are necessary for measuring the symmetry-protected BICs, the off- Γ (accidental) BICs demonstrated in **Figure 5-1** as well as the symmetry-breaking BICs demonstrated in **Figures 5-5** and **5-6**.

5.6 conclusion

We have proposed a class of metasurfaces composed of orthogonally arranged dielectric bars for observation of BICs in terahertz regime. The metasurface with symmetry of C_{4v} point group demonstrate the well-known symmetry-protected BICs at the Γ point for both TM_1 and TM_2 bands. Moreover, the TM_2 band also shows off- Γ BICs at unpredicted in-plane wavevectors. By breaking the in-plane symmetry, additional BICs have been observed and the physical insights have been fully discussed. Moreover, the symmetry-broken BICs observed experimentally are quasi-states that support highly confined electromagnetic fields, both inside and outside of the dielectric metasurfaces. Therefore, the proposed system is promising for many real-world applications.

Chapter 6: Dynamic bound states in the continuum in zero-index photonic crystal slab

6.1 Introduction

Artificially tailoring the EM parameters of materials to arbitrary manipulate EM wave has been the ultimate pursuit since the Maxwell's equations were united for derivation of the wave equation [63-65]. To do so, the basic concept is to engineer the refractive index, given by $n = \sqrt{\epsilon\mu}$, of the material. The response to both electric and magnetic fields of EM wave as quantified by permittivity (ϵ) and permeability (μ) reveals the index of a material [155, 156]. However, for a long period, various optical components were built only on intrinsic properties of natural materials, for example, lenses achieve wave front control through accumulated light paths (phase as well as amplitude) when light propagating inside it. Until the end of last century, PhCs and metamaterials appeared successively that allow scientists, for the first time, to control EM wave at will. Metamaterials, however, manipulate the optical properties of matter with unprecedented flexibility and exotic phenomena, including the ability to access negative index [157-160], cloaking [238-240], and chiral optical properties [178, 195].

During the past decade, there has been significant interests in the near-zero (refractive) index metamaterials and PhCs, inside which wave experiences no spatial phase change [142, 241-246]. Therefore, zero-index metamaterials and PhCs can be applied for directional emission [142], EM cloaks [241], large-area single-mode devices [244] and tunneling waveguides [245]. As indicated by the formula $n = \sqrt{\epsilon\mu}$, a zero-index can be achieved by epsilon-near-zero (ENZ), which is easily realized as metals show ENZ at the ultraviolet plasma frequency [247], metallic waveguides constructed by a pair of parallel plates have ENZ at their cutoff frequency [248], naturally occurring materials such as transparent conducting oxides (TCOs) demonstrate ENZ at optical frequencies [249-251], and metamaterials with negative permittivity have a transition from positive effective permittivity to negative permittivity such that ENZ is the

transition point [142, 241-246, 251-255]. However, a significant limitation of ENZ materials is their mismatched impedance, given by $Z = \sqrt{\mu/\epsilon}$, that causes high reflectivity at the interface, and no waves are therefore allowed to propagate [249-251]. In addition, metals, especially in optical frequencies, suffer high losses and absent isotropy. Therefore, the all-dielectric Dirac-cone zero-index metamaterials (ZIM) have recently emerged as one of canonical solutions for eliminating intrinsic losses [142, 243, 244, 246]. Building block with high-index dielectrics, their responses to EM field for both electric and magnetic resonances governed by Mie theory can be simultaneously excited in such metamaterials and PhCs [142]. As results, both ϵ_{eff} and μ_{eff} can be simultaneously tuned to cross zero for given frequency by carefully tailoring the lattice arrangement, resonator geometry, and material composite [142, 243, 244, 246]. Accidental degeneracy of photonic band structures, which shows the intersection of two linear bands near the Γ point, or a Dirac-like cone, is produced coincident magnetic and electric resonances [142, 243, 244, 246]. The Dirac dispersion is analogous to the electronic dispersion of graphene, an atomic lattice with hexagon array, which features as the linear band crossing at the K/K' point of the Brillouin zone. By constructing the Dirac-cone for ZIMs with dielectrics, the device not only eliminates the intrinsic losses associated with metals, but also possesses finite impedance that enables wave coupling with integrated photonics, which is especially important for CMOS compatible integrated applications [244, 246].

Just like the terahertz known as a “gap”, low-loss Dirac-cone ZIMs is also blank in this regime. However, terahertz technologies are expected to meet the ever-increasing demand for extremely high-speed wireless communications [31, 32]. Most recently, it has been shown that terahertz topological photonics process low-loss, high-capacity, high-speed and robust on-chip communications [256]. However, topological photonics contain bulk footprints such that it's hard for them to be highly integrated. By constricting dielectric Dirac-cone ZIMs, the exact fingerprint of device becomes irrelevant such that they may have a chance to be highly

compatible for terahertz communications. To eliminate the radiation loss, a Dirac-cone zero-index BICs has been recently proposed to enable the extremely low radiating loss to be 1 dB/mm in theory [257].

In this chapter, we follow the recently reported concept of zero-index BICs at photonic Dirac cone. The angle-resolved far-field measurements were done by using THz-TDS. The scan length has been extremely extended, for the first time, to be 800 ps for the employed THz-TDS. Further, the zero-index PhC slab was actively modulated by introducing near infrared laser pump. Therefore, we realized an active modulation of zero-index PhC slab that would find plenty of application, for example terahertz on-chip comb for communications.

6.2 Design and fabrication

A hexagonal lattice with a C_{6v} point group is considered, as shown in **Figure 6-1**. The air holes are drilled through a silicon ($n_{Si} = 3.48$) slab with lattice period $\Lambda = 400 \mu\text{m}$ thickness of $t = 0.5\Lambda$. The holes have a 3-fold rotation of an ellipse with long axis of $a = 344 \mu\text{m}$ and short axis $b = 128 \mu\text{m}$. According to ref. [257], this photonic structure is referred as a “daisy” PhC slab. The optical imaged of unetched sample is shown in **Figure 6-1(a)**, where green color is the photoresist and purple patterns are the SiO_2 layer. The SEM image of fabricated sample is shown in **Figure 6-1(b)**, which will be measured with angle-resolved far-field THz-TDS.

To fabricate the sample, we employed a four-step lithography and etching process to create the PhC slab.

- (1) SiO_2 Deposition. A SiO_2 with thickness of $2 \mu\text{m}$ was deposited on the cleaned high-resistivity silicon ($>10000 \Omega\cdot\text{cm}$) wafer with thickness of $200 \mu\text{m}$ by the PECVD.
- (2) Spin-coating photoresist on the SiO_2 /silicon hybrid wafer. The AZ 5214E photoresist was spin coated on the SiO_2 /silicon hybrid wafer with spin speed of 6000 rpm for 45 s with acceleration deceleration time is 5 s and deceleration time is 5 s, which make sure

the thickness of photoresist is larger than $1.2\ \mu\text{m}$. To solidify the photoresist, the photoresist-coated samples are baking for 2 mins on hot-plate with temperature of $110\ ^\circ\text{C}$.

(3) Mask-free UV lithography for Patterning daisy structures on photoresist. The hybrid photoresist-coated SiO_2 -on-silicon wafer is patterned by Microwriter ML®3 (405 nm long-life semiconductor LED light source) from Durham Magneto Optics Ltd. The writing speed is up to $20\ \text{mm}^2/\text{minute}$. The lithography has $1\ \mu\text{m}$ resolution across full writing area. After photolithography, the UV illuminated photoresist is removed by using 351B developer for about 35 s following by a 15 s DI water clean.

(4) The SiO_2 was removed by the RIE and the silicon was etched by the DRIE with receipt same as **Chapter 3**.

Figure 6-1. Design of terahertz daisy PhC slab for Dirac-cone zero-index BICs. (a) Optical image of the samples before etching. Black hexagon with horizontal width of $\Lambda = 400\ \mu\text{m}$ shows the C_{6v} lattice, and cyan hexagon indicates the reciprocal lattice. The daisy patterns are formed by 3-fold rotating an ellipse with long axis of $a = 344\ \mu\text{m}$ and short axis of $b = 128\ \mu\text{m}$. (b) SEM image of the fabricated sample after etching. The sample is air holes drilled through silicon slab with thickness of $t = 200\ \mu\text{m}$.

6.3 Point-group symmetry analysis

To understand the Dirac-cone band structure at the Γ -point of the daisy PhC slab, the point-group analysis is necessary. The band structure, field profile and Q -factors of each band are calculated by the finite element method of COMSOL Multiphysics, where the quasi-TM band structure is shown in **Figure 6-2**. The photonic band structure shows a Dirac-like cone at around 0.3643 THz, where a 3-fold degeneracy is observed. With the 2D periodic PhC structure, at least one 2D irreducible representation is supported by the point-group symmetry. At the Γ point, the PhC slab supports a singly degenerated state $|S\rangle$ at a frequency of ω_1 , and a pair of doubly degenerated states $|p_x\rangle$ and $|p_y\rangle$ that belong to the 2D irreducible representation at a frequency of ω_2 . The accidental degeneracy says $\omega_1 = \omega_2$. In the vicinity of the Γ point, the band structure of the PhC slab is described, using the $k \cdot p$ method for the first order, by an effective Hamiltonian [258]:

$$C_k = \begin{pmatrix} 0 & 0 & b_x k_x \\ 0 & 0 & b_y k_y \\ b_x^* k_x & b_y^* k_y & 0 \end{pmatrix}, \quad (6.1)$$

where the b_x and b_y coefficients are given by an overlapping integral between the $|S\rangle$ and $|p_{x/y}\rangle$ states as well as the momentum term, also b_x equals to b_y . The Dirac-like dispersion and a flat band for such Hamiltonian is revealed near the Γ point. This is the same band structure as that of a zero-index material [259]. It has been shown that the effective-medium theory (EMT) can still be formally applied once the Bloch vector $\mathbf{k}$ is close to zero, i.e. when the large effective wavelength is applicable, although the fact is that the elementary cell of the PhC is of comparable size to the free-space wavelength [243, 244]. Therefore, an effective zero-index can be constructed using a PhC slab with an appropriate accidental band degeneracy at the Γ point. Here the hexagonal lattice is a C_{6v} point group such that the 2D irreducible representations denoted as E_1 and E_2 , respectively. Moreover, the modes that belong to the E_2 doesn't couple to the external plane wave at the Γ point, which means the modes are symmetry-

protected BICs. In present system, a nonradiative zero-index BIC can be constructed by forcing an accidental band degeneracy between modes in the E_2 and the B_1 or B_2 irreducible representations, since the $B_{x/y}$ coefficients in Eq. (6.1) in this case are nonzero [257].

Figure 6-2. Eigenmode analysis of terahertz “daisy” PhC slab. (a) and (b) the TM-polarized band shows 3-fold degenerated Dirac cone, and the corresponding Q -factors show symmetry-protected BICs at the Γ point. (c)-(e) The mode profiles at the degenerated Dirac cone. (c) and (d) $B_{x/y}$ representations at 0.3659 THz. (e) E presentation at 0.3643 THz.

The mode profiles of the 3-fold degeneracy band at Γ point are shown in **Figures 6-2(c) to 6-2(e)**, which show the accidental band degeneracy between modes of the E_2 and the B_1 or B_2

irreducible representations. Correspondingly, the Q -factors for each band were also calculated, as shown in **Figure 6-2(b)**. The Q -factors for all three bands diverge at Γ , indicating that they are BIC natures, i.e. fully bundled and coexist with the radiation continuum (above light cone). An additional BIC for the upper band is also observed at $k_x =$ along the ΓK direction. As shown in **Figure 6-2(a)**, the 3-fold degenerated bands can enter the region below light cone such that the guided condition is automatically satisfied resulting in the divergence of Q -factors.

6.4 Zero-index on photonic Dirac cone

To show the zero-index characteristic, we investigate the in-plane phase evolution of the out-of-plane electric field (E_z) in a PhC slab with finite length introduced to it, as shown in **Figure 6-3(a)**. **Figures 6-3(a) to 6-3(c)** show the PhC slab with propagation along the ΓM direction. The periodic boundary conditions were set at $x = \pm\Lambda/2$, and the PML conditions were set in the y and z directions. In the z direction, the PhC was placed at the middle with the PLM condition setting at distance of $3*\Lambda$ from each side of the slab. The excitation frequency is $\bar{\omega} = \omega\Lambda/(2\pi c)$ that is very close to the frequency ω_0 at the Dirac cone, as shown in **Figure 6-3(b)**, where an effectively zero-index response is expected. Indeed, the field is observed as in-phase oscillation for all the elementary cells along the ΓM direction (y -direction). This is the zero-index signature of wave propagation in a PhC slab. However, the phase oscillation along the propagation direction shows slow evolution when the excitation frequency is slightly detuned away from ω_0 , as shown in **Figures 6-3(a) and 6-3(c)**. The phases at equivalent reference points in each elementary cell are plotted in **Figures 6-3(d)**, where it is clearly observed that shows almost zero expansion of phase oscillation at the Dirac cone. It is also observed that the phases vary almost linearly as a function of propagation distance once frequency is slightly tuned away from the Dirac cone. For a homogeneous material with given refractive index n , the field propagation of a planewave follows $E_z(\rho) = E_z(0)e^{ink_0\rho}$, where ρ is the propagation distance, and $k_0 = \omega/c$. Therefore, an effective refractive index n_e can be unambiguously

extracted from the slope of the phase evolutions plotted in **Figure 6-3(d)**, using the model $E_z(y_0 + m\Lambda\sqrt{3}) = E_z(0)e^{in_e k_0 m\Lambda\sqrt{3}}$, with m an integer. **Figure 6-3(e)** shows the calculated effective index that agrees very well the effective index $n'_e = ck/\omega_k$, as obtained by directly calculating the band structure from **Figure 6-2**. Therefore, the band structure in **Figure 6-2** explains very well the field evolution behavior, including the zero-index behavior in a finite-sized PhC structure.

Figure 6-3. (a)-(c) Real parts of the electric field at the middle plane of the PhC slab ($z = 0$) with planewave with a vector along the y -direction (ΓM) exciting from left, at different frequencies $\bar{\omega}$ (a) 0.4857 (0.3639 THz), (b) 0.4861 (Dirac cone, 0.3643 THz), and (c) 0.4870 (0.3650 THz). (d) Phase of E_z at the sampling points marked with blue green dots in the down panels of (a)-(c). (e) Effective index calculated from the phase slope at the given position (black circles), as well as from the Bloch band structure (purple line).

6.5 Terahertz angle-resolved time-domain measurements

6.5.1 TE-polarized far field terahertz measurements

ZnTe-based THz-TDS system with only *TE-polarization* was employed to characterize the transmission spectra. We knew that the spectral resolution of THz-TDS is limited by the scan length of the time-domain pulse (i.e. Chapter 3). To achieve better resolution for probing high- Q resonances, the time-domain pulse must be scanned as longer as possible. However, both the crystal thicknesses of the $\langle 110 \rangle$ ZnTe detector and sample substrate (see **Figure 4-2(c)** in chapter 4) can introduce echo signals to the valid signal that carries high- Q resonance. Here, the sample is substrate free such that the only concern is the echo signal from detector. To avoid it, we attached a 2 mm-thick $\langle 100 \rangle$ ZnTe (not response to the terahertz signal but has same refractive index as the detector) to the $\langle 110 \rangle$ ZnTe detector that allows us to scan 800 ps time-domain pulse (equals to 1.25 GHz spectral resolution), as shown in **Figure 6-4(a)**. The Fourier transformed transmission spectra normalized to the dry nitrogen for three samples are shown in **Figure 6-4(b)**, where the transmissions show slight difference due to the etching of silicon slab was not fully drilled through. Therefore, more stable fabrication is required for future fabrication on in-plane zero-index measurement. Moreover, the continuous steps indicted by black arrow show the Fabry-Perot (FP) interference. In fact, the refractive index of ZnTe is around 3.2 such that 2 mm-thick $\langle 100 \rangle$ crystal only delays the first echo (FP mode in frequency-domain transmission) by 42.7 ps. Obviously, the extremely long scan of terahertz pulse is desirable if the first echo signal is approaching the nose level of THz-TDS system. However, the FP resonance is obvious. As results, the scan length duration is the trade-off between the scan length (resolution) and the number FP interference. To reduce the FP interference and achieve better resonances, we reduce the scan length to 400 ps (2.5 GHz spectra resolution), which will allow us to resolve more distinct resonances.

Figure 6-4. Experimental measurements on fabricated samples. (a) The terahertz scan length in logscale with maximum delay time of 800 picoseconds. (b) The transmission spectra for three samples, where the Fourier transformed spectra in frequency domain are normalized to the dry nitrogen.

Figure 6-5. Numerical simulations and experimental measurements. (a) *TE-polarized* transmission map as function of in-plane wavevector (i.e. angle of incidence). (b) Angle-resolved THz-TDS measurements.

To compare the experiments and numerical calculations, the angle-resolved spectra were measured by rotating the samples, as shown in **Figure 6-5**. The TE-polarized transmission map as function of in-plane wavevector is plotted with frequency ranging from 0.3 THz to 0.5 THz,

as shown in **Figures 6-5(a)**. Six resonances are recognized in **Figure 6-5(a)** that are labelled by ① to ⑥ from lower to higher frequencies. The measured transmission spectra are shown in **Figure 6-5(b)**. It is clearly shown that only resonance modes ② to ⑤ can be observed in the experimental spectra. Due to their extremely high- Q and small amplitude characteristics, the resonance modes ① and ⑥ are not resolved. Therefore, these two modes are easily overwhelmed by the limited scan length (800 picoseconds) and the low signal-loss of the THz-TDS. The terahertz polarizer is necessary for measuring the TE- and TM-polarized transmission spectra.

6.5.2 Dynamic zero-index PhC

Following the OPTP approach in **Chapter 3**, we will experimentally demonstrate an all-optical active modulation of the zero-index PhC slab. An 800-nm femtosecond laser pulse (repetition of 1 kHz, pulse width of 100 fs) is employed to pump zero-index PhC slab. It carries photon energy of 1.55 eV that is larger than the silicon electronic bandgap of 1.1 eV. Therefore, the free carriers can be optically excited with a penetration depth around 10 μm that enable the change of conductivity on the surface of silicon slab [193]. As shown in **Figure 6-6(a)**, the resonant intensity and Q -factors of the transmission spectra are continuously modulated by gradually increasing the photoexcitation pump fluence. The transmission maximum gradually diminishes as the pump fluence continuously increases, and the resonances are fully switched off until 464 $\mu\text{J}/\text{cm}^2$. Once photoexcitation impinges on the samples, the change of silicon conductivity on the surface due to the photo-induced free charge carriers strongly damps the sharp resonance of the PhC slab and finally switches off them upon increased pump fluence. As the pump fluence is further increased, a large number of photo-carriers damps the broadened resonance features that is revealed by the flattened transmission, which will not be totally reflected due to the wide holes drilled inside silicon wafer forming PhC slab. **Figure 6-6(b)** shows the simulated transmission as a function of silicon conductivity (from 0 to 3000 S/m).

It agrees well with the experimental measurements. However, more explorations on the true conductivity of optically pumped silicon are necessary.

Figure 6-6. Active control of zero-index PhC slab with OPTP. (a) Experimental measurements on the transmission spectra as function of pump fluence. (b) Numerical simulations for transmission spectra as function of given conductivity.

6.5.3 Experimental proposal for measuring zero-index bound states in the continuum

As a final demonstration of this work, we investigate the zero-index phenomenon in the “daisy” PhC structure that is finite triangular shape in the in-plane dimensions. The plot in **Figure 6-7(a)** shows the emission from an electric dipole source placed in the middle of the PhC triangular region, surrounded by uniform silicon slab. The dipole frequency is set at the Dirac point, i.e. $\bar{\omega} = 0.4681$. As indicated by previous section, zero-index propagation requests that all the unit cells oscillate in-phase in the “daisy” PhC slab. This leads to highly directional, collimated emission from the interfaces between the PhC slab and the uniform silicon slab. However, it is hard to be experimentally measured as it seems hard to put dipole source inside the silicon region of the PhC structure. The same structure as **Figure 6-7(a)** is now illuminated by a Gaussian beam from the lower side of the uniform silicon slab, as shown in **Figure 6-7(b)**. It is also observed that the outgoing waves in the two above uniform slab regions are similar to that of **Figure 6-7(a)**. For both cases, the in-plane wave propagation of the PhC slab indicates

that once the photonic zero-index mode is excited, it is almost non-radiative without negligible coupling to the surrounding environment. However, the second case is better suitable for real experimental design. Guided mode couplers can be design for coupling in-plane guided wave and out-of-plane detections. Therefore, the transmitted coefficient S_{21} should equal to S_{31} for a zero-index PhC.

Figure 6-7. Real parts of the electric field for a triangular zero-index PhC region surrounded by uniform silicon slab. (a) Dipole source excitation in the center of the PhC region at frequency $\bar{\omega} = \omega\Lambda/(2\pi c) = 0.4861$, and (b) planewave excitation at the bottom of the triangle PhC where the wave propagates along the up direction.

6.6 Conclusion

In summary, we have numerically analyzed a low-loss zero-index BIC in terahertz regime. We have employed long-scan and angle-resolved terahertz measurement to detect the far-field transmission. We claim that more measurements with high resolution terahertz spectroscopy to probe the BICs. Further, we actively control the BIC with optical-pump terahertz probe spectroscopy. We further indicate that the in-plane measurement is necessary, which we'll keep pursuing them for terahertz comb generation and on-chip communication.

Chapter 7: Conclusion and outlooks

In this thesis, we have investigated diverse dielectric metasurfaces and PhC slabs for observation of diverse BICs in terahertz regime. The BICs are non-radiating eigenstates coexisting with radiation continuum of free propagating wave. The localized field for such eigenstates are highly enhanced even they fall into quasi-BIC region. With enhanced field localization, many desired applications due to strong light-matter interaction, such as lasing, high-harmonic generation, and advanced bio-/chemical sensing, et al., can be realized upon scaled sizes of the metasurfaces and PhC slabs. Several initial results have been demonstrated on this journey of probing the exotic behavior of resonant dielectrics. Here, I will summarize these findings as well as outline several promising research directions in the field of BICs in dielectric metamaterials and PhCs.

7.1 Conclusion

Chapter 2 developed the rigorous coupled wave analysis (RCWA), which is one of the best efficient simulation methods. Comparing to the commercial software, such as CST, COMSOL, and FDTD, the RCWA algorithm saves a lot of time as it's meshless characteristic.

Chapters 3 and **Chapter 4** demonstrated 2D dielectric metasurfaces. Under TE-polarized excitation, **Chapter 3** presented an active control of terahertz silicon metasurfaces that support high- Q supercavity in the vicinity of the BIC states. Two BIC regions were recognized by simply tailoring the geometrical length of the silicon resonators, which are revealed as the *resonance-trapped BICs*. Further, the dynamic switching and modulation of the all-dielectric metadvice were shown at extremely low fluence of pump light. Finally, a sub-gigahertz switching speed of the proposed all-optical active metadvice was demonstrated by carefully analyzing the temporal spectral evolution of the supercavity resonance. Under TM-polarized illumination, the metasurface shows two counterpropagating GMR modes at the oblique

incidence. The spectral difference (frequency) between two GMRs at same order increases at larger angles of incidence. However, at very small angles of incidence ($0^\circ < |\theta| \leq 1^\circ$), the destructive interference between two counter-propagating modes (± 1 -order GMRs) enable extremely high- Q resonances that eventually leads to a symmetry-protected BICs with infinite Q -factor at the normal incidence. Our results present the first experimental observation of terahertz GMRs in 2D all-dielectric metasurfaces.

Chapter 5 introduced the in-plane symmetry breaking of a C_{4v} rotationally symmetric lattice. Without breaking the C_{4v} symmetry, the metasurface demonstrate the well-known symmetry-protected BICs at Γ -point. While away from the Γ point, these symmetry-protected BICs transform into quasi-BICs. Moreover, four accidental (off- Γ) BICs were also observed at unpredictable in-plane wavevectors. By breaking the in-plane symmetry, new BICs have been observed. The physics insights have been fully discussed to show that they belong to neither symmetry-protected nor accidental BICs. We therefore defined them as the symmetry-breaking BICs. Their quasi-BICs support highly confined EM fields for both inside and outside of the dielectric metasurfaces, which is promising for local field enhanced applications.

Chapter 6 discussed the low-loss zero-index PhC slab with daisy patterns drilled in a C_{6v} lattice. The non-radiating eigenstates, i.e. BICs, were achieved such that both material loss (silicon) and radiative losses are minimized. Therefore, the in-pane propagating loss can be as small as 1 dB/mm in theory. We did the angle-resoled far field measurements, for the first time, with time-domain scan length of 800 picoseconds. Further, the zero-index BICs were actively modulated with femtosecond pulse pump.

7.2 Outlooks

Strong wave localization in resonant micro-nanostructures is crucial in science and technology. A few directions worth exploring in the future include the following:

First, we believe that terahertz technologies are attracting a lot of attention to cater to the challenges of meeting ever-increasing demand for high-speed wireless communications, among which photonics technologies have played a key role in the development of first-age terahertz communication systems [256]. Therefore, terahertz GMR devices could play a crucial role in communication applications due to its capability for constructing polarizers, beam splitters, differentiators, integrators, and wavelength division (de)multiplexers [199].

Second, the in-plane symmetry breaking metasurfaces have demonstrated to enable enhancement of field localization for both inside and outside the structures. Therefore, they are desirable for advanced bio-/chemical sensors. Symmetry breaking induced BIC or quasi-BIC is irrelevant to the thickness of the structures such that they could be fabricated into ultrathin dielectric metasurfaces. Integrated with gain materials, the highly confined field inside the structure is promising for low threshold lasing upon scale down the structure size to nanoscale. Silicon is one of the most common nonlinear materials. Therefore, we believe the proposed metasurfaces in nanostructure will enhance the high harmonic generations [95]. Without size scaling, these designs are also promising for terahertz quantum cascade lasers (QCLs).

Finally, we believe that the zero-index BICs are the ultimate solution for terahertz combs. A single mode is strictly selected by the geometric design such that different modes can be spatially arranged to form the desired frequency comb. Therefore, this comb could be applied for the next generation on-chip communications. The spatial decoupling characteristics of zero-index materials allow them to be highly compatible. Therefore, the minimum number of the unit cell is also worth to be explored. Once again, the zero-index BICs are also promising for terahertz QCLs.

Appendix I: Publication list

❖ Journal publications during PhD candidature

1. S. Han, L. Cong, H. Lin, B. Xiao, H. Yang, R. Singh. “Tunable electromagnetically induced transparency in coupled three-dimensional split-ring-resonator metamaterials.” *Scientific Reports* 6, 20801 (2016).
2. S. Han, L. Cong, F. Gao, R. Singh, H. Yang. “Observation of Fano resonance and classical analog of electromagnetically induced transparency in toroidal metamaterials.” *Annalen der Physik* 528 (5), 352-357 (2016).
3. S. Han, M. Gupta, L. Cong, Y. K. Srivastava, R. Singh. “Toroidal and magnetic Fano resonances in planar Terahertz metamaterials.” *Journal of Applied Physics* 122 (11), 113105 (2017).
4. S. Han, L. Cong, Y. K. Srivastava, B. Qiang, M. V. Rybin, A. Kumar, R. Jain, W. X. Lim, V. G. Achanta, S. S. Prabhu, Q. Wang, Y. S. Kivshar, R. Singh. “All-Dielectric Active Terahertz Photonics Driven by Bound States in the Continuum.” *Advanced Materials* 31 (37), 1901921 (2019).
5. S. Han, M. V. Rybin, P. Pitchappa, Y. K. Srivastava, Y. S. Kivshar, and R. Singh. “Guided-mode resonances in all-dielectric terahertz metasurfaces.” *Advanced Optical Materials* 1900959 (2019).

❖ Collaborative publications

1. H. Lin, D. Yang, S. Han, Y. Liu, and H. Yang. “Analog electromagnetically induced transparency for circularly polarized wave using three-dimensional chiral metamaterials” *Optics express* 24 (26), 30068-30078 (2016).
2. W. X. Lim, S. Han, M. Gupta, K. F. MacDonald, R. Singh. “Near-infrared linewidth narrowing in plasmonic Fano-resonant metamaterials via tuning of multipole contributions.” *Applied Physics Letters* 111 (6), 061104 (2017).

3. K. V. Sreekanth, S. Sreejith, S. Han, A. Mishra, X. Chen, H. Sun, C. T. Lim, R. Singh. "Biosensing with the singular phase of an ultrathin metal-dielectric nanophotonic cavity." *Nature communications* 9 (1), 369 (2018).
4. K. V. Sreekanth, Q. Ouyang, S. Han, K. T. Yong, R. Singh. "Giant enhancement in Goos-Hänchen shift at the singular phase of a nanophotonic cavity." *Applied Physics Letters* 112 (16), 161109 (2018).
5. K. V. Sreekanth, S. Han, R. Singh. "Ge₂Sb₂Te₅ - Based Tunable Perfect Absorber Cavity with Phase Singularity at Visible Frequencies." *Advanced Materials* 30 (21), 1706696 (2018).
6. E. Bochkova, S. Han, A. de Lustrac, R. Singh, S. N. Burokur, A. Lupu. "High-Q Fano resonances via direct excitation of an antisymmetric dark mode." *Optics Letters* 43 (16), 3818-3821 (2018).
7. L. Cong, V. Savinov, Y. K. Srivastava, S. Han, R. Singh. "A metamaterial analog of the Ising model." *Advanced Materials* 30 (40), 1804210 (2018).
8. K. V. Sreekanth, P. Mahalakshmi, S. Han, M. S. M. Rajan, P. K. Choudhury, R. Singh. "Brewster Mode - Enhanced Sensing with Hyperbolic Metamaterial." *Advanced Optical Materials* 7 (21), 1900680 (2019).

Bibliography

- [1]. Siegel, P. H. Terahertz technology. *IEEE Trans. Microwave Theory Tech.* 50, 910 (2002).
- [2]. Williams, G. P. Filling the THz gap—high power sources and applications. *Rep. Prog. Phys.* 69, 301 (2006).
- [3]. Tao, H. et al. Recent progress in electromagnetic metamaterial devices for terahertz applications. *IEEE J. Selected Topics Quantum Electron.* 17, 92 (2011).
- [4]. Tonouchi, M. Cutting-edge terahertz technology. *Nat. Photonics* 1, 97 (2007).
- [5]. Lee, Y. S. *Principles of terahertz science and technology* (Vol. 170). Springer Science & Business Media (2009).
- [6]. Rostami, A. et al. *Terahertz technology: fundamentals and applications* (Vol. 77). Springer Science & Business Media (2010).
- [7]. Ferguson, B. & Zhang, X. C. Materials for terahertz science and technology. *Nat. Mater.* 1, 26 (2002).
- [8]. Beard, M. C. et al. Terahertz spectroscopy. *J. Phys. Chem. B* 106, 7146 (2002).
- [9]. Williams, B. S. Terahertz quantum-cascade lasers. *Nat. photonics*, 1, 517 (2007).
- [10]. Hoffmann, M. C. & Fülöp, J. A. Intense ultrashort terahertz pulses: generation and applications. *J. Phys. D: Appl. Phys.* 44, 083001 (2011).
- [11]. Zouaghi, W. et al. Broadband terahertz spectroscopy: principles, fundamental research and potential for industrial applications. *Eur. J. Phys.* 34, S179 (2013).
- [12]. Sirtori, C. et al. Wave engineering with THz quantum cascade lasers. *Nat. Photonics* 7, 691 (2013).
- [13]. Lewis, R. A. A review of terahertz sources. *J. Phys. D: Appl. Phys.* 47, 374001 (2014).
- [14]. Hangyo, M. Development and future prospects of terahertz technology. *Jpn. J. Appl. Phys.* 54, 120101 (2015).

- [15]. Pawar, A. Y. et al. Terahertz technology and its applications. *Drug Discov. Today* 5, 157 (2013).
- [16]. Hafez, H. A. et al. Intense terahertz radiation and their applications. *J. Opt.* 18, 093004 (2016).
- [17]. Dhillon, S. S. et al. The 2017 terahertz science and technology roadmap. *J. Phys. D: Appl. Phys.* 50, 043001 (2017).
- [18]. Ropagnol, X. et al. Intense terahertz generation at low frequencies using an interdigitated ZnSe large aperture photoconductive antenna. *Appl. Phys. Lett.* 103, 161108 (2013).
- [19]. Aoki, K. et al. Broadband terahertz pulse generation by optical rectification in GaP crystals. *Appl. Phys. Lett.* 110, 201103 (2017).
- [20]. Ruchert, C. et al. Scaling submillimeter single-cycle transients toward megavolts per centimeter field strength via optical rectification in the organic crystal OH1. *Opt. Lett.* 37, 899 (2012).
- [21]. Hauri, C. P. et al. Strong-field single-cycle THz pulses generated in an organic crystal. *Appl. Phys. Lett.* 99, 161116 (2011).
- [22]. Vicario, C. et al. GV/m single-cycle terahertz fields from a laser-driven large-size partitioned organic crystal. *Phys. Rev. Lett.* 112, 213901 (2014).
- [23]. Seifert, T. et al. Efficient metallic spintronic emitters of ultrabroadband terahertz radiation. *Nat. Photonics* 10, 483 (2016).
- [24]. Walowski, J. & Münzenberg, M. Perspective: Ultrafast magnetism and THz spintronics. *J. Appl. Phys.* 120, 140901 (2016).
- [25]. Palfalvi, L. et al. Nonlinear refraction and absorption of Mg doped stoichiometric and congruent LiNbO₃. *J. Appl. Phys.* 95, 902 (2004).

- [26]. Palfalvi, L. et al. Temperature dependence of the absorption and refraction of Mg-doped congruent and stoichiometric LiNbO₃ in the THz range. *J. Appl. Phys.* 97, 123505 (2005).
- [27]. Hirori, H. et al. Single-cycle terahertz pulses with amplitudes exceeding 1 MV cm⁻¹ generated by optical rectification in LiNbO₃. *Appl. Phys. Lett.* 98, 091106 (2011).
- [28]. Deninger, A. J. et al. 2.75 THz tuning with a triple-DFB laser system at 1550 nm and InGaAs photomixers. *J. Infrared Millim. Terahertz Waves* 36, 269 (2015).
- [29]. Ulbricht, R. et al. Carrier dynamics in semiconductors studied with time-resolved terahertz spectroscopy. *Rev. Mod. Phys.* 83, 543 (2011).
- [30]. Kampfrath, T. et al. Resonant and nonresonant control over matter and light by intense terahertz transients. *Nat. Photonics* 7, 680 (2013).
- [31]. Federici, J. & Moeller, L. Review of terahertz and subterahertz wireless communications. *J. Appl. Phys.* 107, 6 (2010).
- [32]. Nagatsuma, T. et al. Advances in terahertz communications accelerated by photonics. *Nat. Photonics* 10, 371 (2016).
- [33]. Mittleman, D. M. et al. Recent advances in terahertz imaging. *Appl. Phys. B* 68, 1085 (1999).
- [34]. Federici, J. F. et al. THz imaging and sensing for security applications—explosives, weapons and drugs. *Semicond. Sci. Technol.* 20, S266 (2005).
- [35]. Karpowicz, N. et al. Comparison between pulsed terahertz time-domain imaging and continuous wave terahertz imaging. *Semicond. Sci. Technol.* 20, S293 (2005).
- [36]. Chan, W. L. et al. Imaging with terahertz radiation. *Rep. Prog. Phys.* 70, 1325 (2007).
- [37]. Karpowicz, N. et al. Compact continuous-wave subterahertz system for inspection applications. *Appl. Phys. Lett.* 86, 054105 (2005).
- [38]. Ruggiero, M. T. et al. Measuring the Elasticity of Poly - l - Proline Helices with Terahertz Spectroscopy. *Angew. Chem.* 55, 6877 (2016).

- [39]. Korter, T. M. & Plusquellic, D. F. Continuous-wave terahertz spectroscopy of biotin: vibrational anharmonicity in the far-infrared. *Che. Phys. Lett.* 385, 45 (2004).
- [40]. Woodward, R. M. Terahertz pulse imaging of ex vivo basal cell carcinoma. *J. Investig. Dermatol.* 120, 72 (2003).
- [41]. Han, P. Y. et al. Time-domain transillumination of biological tissues with terahertz pulses. *Opt. Lett.* 25, 242 (2000).
- [42]. Kawase, K. et al. Non-destructive terahertz imaging of illicit drugs using spectral fingerprints. *Opt. Express* 11, 2549 (2003).
- [43]. Floquet, G. Sur les équations différentielles linéaires à coefficients périodiques. *Annales Scientifiques de l'École Normale Supérieure* 12, 47 (1883).
- [44]. Joannopoulos, J. D. Photonic crystals. *Solid State Commun.* 102, 165 (1997).
- [45]. Sakoda, K. Optical properties of photonic crystals (Vol. 80). Springer Science & Business Media (2004).
- [46]. Joannopoulos, J. D. et al. Molding the flow of light. Princeton Univ. Press, Princeton, NJ (2008).
- [47]. Rayleigh, L. XXV. On copying diffraction-gratings, and on some phenomena connected therewith. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 11, 196 (1881).
- [48]. Inoue, K. & Ohtaka, K. Photonic crystals: physics, fabrication and applications (Vol. 94). Springer Science & Business Media (2004).
- [49]. Massaro, A. Photonic Crystals: Introduction, Applications and Theory. BoD—Books on Demand (2012).
- [50]. Gong, Q. & Hu, X. Photonic crystals: principles and applications. Jenny Stanford Publishing (2014).

- [51]. Fan, S. & Joannopoulos, J. D. Analysis of guided resonances in photonic crystal slabs. *Phys. Rev. B* 65, 235112 (2002).
- [52]. Korkin, A. & Rosei, F. Nanoelectronics and photonics: from atoms to materials, devices, and architectures. Springer Science & Business Media (2008).
- [53]. Foley, J. M. et al. Symmetry-protected mode coupling near normal incidence for narrow-band transmission filtering in a dielectric grating. *Phys. Rev. B* 89, 165111 (2014).
- [54]. Jamois, C. et al. Silicon-based two-dimensional photonic crystal waveguides. *Photonics Nanostructures: Fundam. Appl.* 1, 1 (2003).
- [55]. Wood, R. W. On a remarkable case of uneven distribution of light in a diffraction grating spectrum. *Philos. Mag.* 4, 396 (1902).
- [56]. Rayleigh, L. Note on the remarkable case of diffraction spectra described by Prof. Wood. *Philos. Mag.* 14, 60 (1907)
- [57]. Rayleigh, L. On the dynamical theory of gratings. *Proc. R. Soc. Lond.* 79, 399 (1907).
- [58]. von Neumann, J. & Wigner, E. Über merkwürdige diskrete Eigenwerte. *Phys. Z.* 30, 465 (in German) (1929).
- [59]. Parker, R. Resonance effects in wake shedding from parallel plates: some experimental observations. *J. Sound Vib.* 4, 62 (1966).
- [60]. Parker, R. Resonance effects in wake shedding from parallel plates: calculation of resonant frequencies. *J. Sound Vib.* 5, 330 (1967).
- [61]. Cumpsty, N. A. & Whitehead, D. S. The excitation of acoustic resonances by vortex shedding. *J. Sound Vib.* 18, 353 (1971).
- [62]. Koch, W. Resonant acoustic frequencies of flat plate cascades. *J. Sound Vib.* 88, 233 (1983).

- [63]. Parker, R. & Stoneman, S. A. T. The excitation and consequences of acoustic resonances in enclosed fluid flow around solid bodies. *Proc. Inst. Mech. Eng. C* 203, 9 (1989).
- [64]. Evans, D. V. et al. Existence theorems for trapped modes. *J. Fluid Mech.* 261, 21 (1994).
- [65]. Evans, D. V. et al. Trapped mode frequencies embedded in the continuous spectrum. *Q. J. Mech. Appl. Math.* 46, 253 (1993).
- [66]. Groves, M. D. Examples of embedded eigenvalues for problems in acoustic waveguides. *Math. Meth. Appl. Sci.* 21, 479 (1998).
- [67]. Linton, C. & McIver, M. Trapped modes in cylindrical waveguides. *Q. J. Mech. Appl. Math.* 51, 389 (1998).
- [68]. Davies, E. & Parnowski, L. Trapped modes in acoustic waveguides. *Q. J. Mech. Appl. Math.* 51, 477 (1998).
- [69]. Ursell, F. Trapping modes in the theory of surface waves. *Math. Proc. Cambridge Philos. Soc.* 47, 347 (1951).
- [70]. Jones, D. S. The eigenvalues of $\nabla^2 u + \lambda u = 0$ when the boundary conditions are given on semi-infinite domains. *Math. Proc. Cambridge Philos. Soc.* 49, 668 (1953).
- [71]. Callan, M. et al. Trapped modes in two-dimensional waveguides. *J. Fluid Mech.* 229, 51 (1991).
- [72]. Retzler, C. H. Trapped modes: an experimental investigation. *Appl. Ocean Res.* 23, 249 (2001).
- [73]. Cobelli, P. J. et al. Experimental observation of trapped modes in a water wave channel. *Euro. Phys. Lett.* 88, 20006 (2009).
- [74]. Cobelli, P. J. et al. Experimental study on water-wave trapped modes. *J. Fluid Mech.* 666, 445 (2011).

- [75]. Schult, R. L. et al. Quantum bound states in a classically unbound system of crossed wires. *Phys. Rev. B* 39, 5476 (1989).
- [76]. Exner, P. et al. Bound states and scattering in quantum waveguides coupled laterally through a boundary window. *J. Math. Phys.* 37, 4867 (1996).
- [77]. Hsu, C. W. et al. Bound states in the continuum. *Nat. Rev. Mater.* 1, 16048 (2016).
- [78]. Marinica, D. C. et al. Bound states in the continuum in photonics. *Phys. Rev. Lett.* 100, 183902 (2008).
- [79]. Plotnik, Y. et al. Experimental observation of optical bound states in the continuum. *Phys. Rev. Lett.* 107, 183901 (2011).
- [80]. Molina, M. I. Surface bound states in the continuum. *Phys. Rev. Lett.* 108, 070401 (2012).
- [81]. Hsu, C. W. et al. Bloch surface eigenstates within the radiation continuum. *Light Sci. Appl.* 2, e84 (2013).
- [82]. Hsu, C. W. et al. Observation of trapped light within the radiation continuum. *Nature* 499, 188 (2013).
- [83]. Yang, Y. Analytical perspective for bound states in the continuum in photonic crystal slabs. *Phys. Rev. Lett.* 113, 037401 (2014).
- [84]. Blanchard, C. et al. Fano resonances in photonic crystal slabs near optical bound states in the continuum. *Phys. Rev. B* 94, 155303 (2016).
- [85]. Gansch, R. et al. Measurement of bound states in the continuum by a detector embedded in a photonic crystal. *Light Sci. Appl.* 5, e16147 (2016).
- [86]. Yuan, L. & Lu, Y. Y. Bound states in the continuum on periodic structures surrounded by strong resonances. *Phys. Rev. A* 97, 043828 (2018).
- [87]. Azzam, S. I. et al. Formation of bound states in the continuum in hybrid plasmonic-photonic systems. *Phys. Rev. Lett.* 121, 253901 (2018).

- [88]. Lee, S. G. & Magnusson, R. Band flips and bound-state transitions in leaky-mode photonic lattices. *Phys. Rev. B* 99, 045304 (2019).
- [89]. Cerjan, A. et al. Bound States in the Continuum through Environmental Design. *Phys. Rev. Lett.* 123, 023902 (2019).
- [90]. Zhen, B. et al. Topological nature of optical bound states in the continuum. *Phys. Rev. Lett.* 113, 257401 (2014).
- [91]. Bulgakov, E. N. & Maksimov, D. N. Bound states in the continuum and polarization singularities in periodic arrays of dielectric rods. *Phys. Rev. A* 96, 063833 (2017).
- [92]. Zhang, Y. et al. Observation of polarization vortices in momentum space. *Phys. Rev. Lett.* 120, 186103 (2018).
- [93]. Doeleman, H. M. et al. Experimental observation of a polarization vortex at an optical bound state in the continuum. *Nat. Photonics* 12, 397 (2018).
- [94]. Carletti, L. et al. Giant nonlinear response at the nanoscale driven by bound states in the continuum. *Phys. Rev. Lett.* 121, 033903 (2018).
- [95]. Liu, H. et al. Enhanced high-harmonic generation from an all-dielectric metasurface. *Nat. Phys.* 14, 1006 (2018).
- [96]. Hirose, K. et al. Watt-class high-power, high-beam-quality photonic-crystal lasers. *Nat. Photonics* 8, 406 (2014).
- [97]. Kodigala, A. et al. Lasing action from photonic bound states in continuum. *Nature* 541, 196 (2017).
- [98]. Tittl, A. et al. Imaging-based molecular barcoding with pixelated dielectric metasurfaces. *Science* 360, 1105 (2018).
- [99]. Leitis, A. et al. Angle-multiplexed all-dielectric metasurfaces for broadband molecular fingerprint retrieval. *Sci. Adv.* 5, eaaw2871 (2019).

- [100]. Yesilkoy, F. et al. Ultrasensitive hyperspectral imaging and biodetection enabled by dielectric metasurfaces. *Nat. Photonics* 13, 390 (2019).
- [101]. Yamanouchi, K. & Shibayama, K. Propagation and amplification of rayleigh waves and piezoelectric leaky surface waves in LiNbO₃. *J. Appl. Phys.* 43, 856 (1972).
- [102]. Kawachi, O. et al. Optimal cut for leaky SAW on LiTaO₃ for high performance resonators and filters. *IEEE Trans. Ultrason. Ferroelectr. Freq. Control* 48, 1442 (2001).
- [103]. Rout, S. & Sonkusale, S. Active metamaterials: terahertz modulators and detectors. Springer (2017).
- [104]. Jiang, Z. & Zhang, X. C. Terahertz imaging via electrooptic effect. *IEEE Trans. Microwave Theory Tech.* 47, 2644 (1999).
- [105]. Watts, C. M. Terahertz compressive imaging with metamaterial spatial light modulators. *Nat. Photonics* 8, 605 (2014).
- [106]. Zheludev, N. I. & Plum, E. Reconfigurable nanomechanical photonic metamaterials. *Nat. Nanotech.* 11, 16 (2016).
- [107]. Driscoll, T. et al. Memory metamaterials. *Science*, 325, 1518 (2009).
- [108]. Tao, H. et al. Reconfigurable terahertz metamaterials. *Physical review letters*, 103, 147401 (2009).
- [109]. Chen, H. T. et al. Tuning the resonance in high-temperature superconducting terahertz metamaterials. *Phys. Rev. Lett.* 105(24), 247402 (2010).
- [110]. Singh, R. et al. Optical tuning and ultrafast dynamics of high-temperature superconducting terahertz metamaterials. *Nanophotonics* 1, 117 (2012).
- [111]. Srivastava, Y. K. et al. A Superconducting Dual-Channel Photonic Switch. *Adv. Mater.* 30, 1801257 (2018).
- [112]. Pitchappa, P. et al. Chalcogenide phase change material for active terahertz photonics. *Adv. Mater.* 31, 1808157 (2019).

- [113]. Pitchappa, P. et al. Active control of electromagnetically induced transparency analog in terahertz MEMS metamaterial. *Adv. Opt. Mater.* 4, 541 (2016).
- [114]. Manjappa, M. et al. Reconfigurable MEMS Fano metasurfaces with multiple-input–output states for logic operations at terahertz frequencies. *Nat. Commun.* 9, 4056 (2018).
- [115]. Shrekenhamer, D. et al. Liquid crystal tunable metamaterial absorber. *Phys. Rev. Lett.* 110, 177403 (2013).
- [116]. Chen, H. T. et al. Active terahertz metamaterial devices. *Nature* 444, 597 (2006).
- [117]. Lee, S. H. et al. Switching terahertz waves with gate-controlled active graphene metamaterials. *Nat. Mater.* 11, 936 (2012).
- [118]. Alius, H. & Dodel, G. Amplitude-, phase-, and frequency modulation of far-infrared radiation by optical excitation of silicon. *Infrared Phys.* 32, 1 (1991).
- [119]. Vogel, T. et al. High-speed switching of far-infrared radiation by photoionization in a semiconductor. *Appl. Opt.* 31(3), 329 (1992).
- [120]. Nozokido, T. et al. Modulation of submillimeter wave radiation by laser produced free carriers in semiconductors. *Electron. Commun. Jpn. (Part II: Electron.)* 80(6), 1 (1997)
- [121]. Hendry, E. et al. Ultrafast optical switching of the THz transmission through metallic subwavelength hole arrays. *Phys. Rev. B* 75, 235305 (2007).
- [122]. Chen, H. T. et al. Ultrafast optical switching of terahertz metamaterials fabricated on ErAs/GaAs nano-island superlattices. *Opt. Lett.* 32, 1620 (2007).
- [123]. Yang, Y. et al. Femtosecond optical polarization switching using a cadmium oxide-based perfect absorber. *Nat. Photonics* 11, 390 (2017).
- [124]. Lim, W. X. et al. Ultrafast All-Optical Switching of Germanium-Based Flexible Metaphotonic Devices. *Adv. Mater.* 30, 1705331 (2018).
- [125]. Shcherbakov, M. R. et al. Ultrafast all-optical tuning of direct-gap semiconductor metasurfaces. *Nat. Commun.* 8, 17 (2017).

- [126]. Moharam, M. G. & Gaylord, T. K. Rigorous coupled-wave analysis of planar-grating diffraction. *JOSA* 71, 811 (1981).
- [127]. Moharam, M. G. & Gaylord, T. K. Diffraction analysis of dielectric surface-relief gratings. *JOSA* 72, 1385 (1982).
- [128]. Moharam, M. G. & Gaylord, T. K. Rigorous coupled-wave analysis of grating diffraction—E-mode polarization and losses. *JOSA* 73, 451 (1983).
- [129]. Moharam, M. G. & Gaylord, T. K. Three-dimensional vector coupled-wave analysis of planar-grating diffraction. *JOSA* 73, 1105 (1983).
- [130]. Gaylord, T. K. & Moharam, M. G. Analysis and applications of optical diffraction by gratings. *Proc. IEEE* 73, 894 (1985).
- [131]. Moharam, M. G. & Gaylord, T. K. Rigorous coupled-wave analysis of metallic surface-relief gratings. *JOSA A* 3, 1780 (1986).
- [132]. Moharam, M. G. et al. Formulation for stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings. *JOSA A* 12, 1068 (1995).
- [133]. Moharam, M. G. et al. Stable implementation of the rigorous coupled-wave analysis for surface-relief gratings: enhanced transmittance matrix approach. *JOSA A* 12, 1077 (1995).
- [134]. Li, L. Use of Fourier series in the analysis of discontinuous periodic structures. *JOSA A* 13, 1870-1876 (1996).
- [135]. Lalanne, P. & Morris, G. M. Highly improved convergence of the coupled-wave method for TM polarization. *JOSA A* 13, 779 (1996).
- [136]. Li, L. Multilayer modal method for diffraction gratings of arbitrary profile, depth, and permittivity. *JOSA A* 10, 2581 (1993).
- [137]. Li, L. Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings. *JOSA A* 13, 1024 (1996).

- [138]. Ko, D. Y. K. & Inkson, J. C. Matrix method for tunneling in heterostructures: Resonant tunneling in multilayer systems. *Phys. Rev. B* 38, 9945 (1988).
- [139]. Whittaker, D. M. & Culshaw, I. S. Scattering-matrix treatment of patterned multilayer photonic structures. *Phys. Rev. B* 60, 2610 (1999).
- [140]. Liscidini, M. et al. Scattering-matrix analysis of periodically patterned multilayers with asymmetric unit cells and birefringent media. *Phys. Rev. B* 77, 035324 (2008).
- [141]. Caballero, B. et al. Generalized scattering-matrix approach for magneto-optics in periodically patterned multilayer systems. *Phys. Rev. B* 85, 245103 (2012).
- [142]. Moitra, P. et al. Realization of an all-dielectric zero-index optical metamaterial. *Nat. Photonics* 7, 791 (2013).
- [143]. Nojonen, E. & Turunen, J. Eigenmode method for electromagnetic synthesis of diffractive elements with three-dimensional profiles. *JOSA A* 11, 2494 (1994).
- [144]. Li, L. New formulation of the Fourier modal method for crossed surface-relief gratings. *JOSA A* 14, 2758 (1997).
- [145]. Chang-Hasnain, C. J. & Yang, W. High-contrast gratings for integrated optoelectronics. *Adv. Opt. Photon.* 4, 379 (2012).
- [146]. Qiao, P. et al. Recent advances in high-contrast metastructures, metasurfaces, and photonic crystals. *Adv. Opt. Photon.* 10, 180 (2018).
- [147]. Richtmyer, R. D. Dielectric resonators. *J. Appl. Phys.* 10, 391-398 (1939).
- [148]. Sethares, J. C. & Naumann, S. J. Design of microwave dielectric resonators. *IEEE Trans. Microw. Theory Tech.* 14, 2-7 (1966).
- [149]. Cohn, S. B. Microwave bandpass filters containing high-Q dielectric resonators. *IEEE Trans. Microw. Theory Tech.* 16, 218-227 (1968).
- [150]. Long, S. McAllister, M. & Shen, L. The resonant cylindrical dielectric cavity antenna. *IEEE Trans. Antennas Propag.* 31, 406-412 (1983).

- [151]. Kajfez, D. & Guillon, P. Dielectric resonators. Artech House: Norwood, MA, 1986.
- [152]. Mongia, R. K. & Bhartia, P. Dielectric resonator antennas—A review and general design relations for resonant frequency and bandwidth. *Int. J. RF Microw. Comput.-Aided Eng.*, 4, 230-247 (1994).
- [153]. Mongia, R. K. & Ittipiboon, A. Theoretical and experimental investigations on rectangular dielectric resonator antennas. *IEEE Trans. Antennas Propag.* 45, 1348-1356 (1997).
- [154]. O'Brien, S. & Pendry, J. B. Photonic band-gap effects and magnetic activity in dielectric composites. *Journal of Physics: Condensed Matter*, 14, 4035 (2002).
- [155]. Veselago, V. G. The electrodynamics of substances with simultaneously negative values of ϵ and μ . *Physics-Uspekhi*, 10, 509 (1968).
- [156]. Pendry, J. B. Negative refraction makes a perfect lens. *Phys. Rev. Lett.* 85, 3966 (2000).
- [157]. Shelby, R. A. et al. Experimental verification of a negative index of refraction. *Science* 292, 77 (2001).
- [158]. Smith, D. R. Metamaterials and negative refractive index. *Science* 305, 788 (2004).
- [159]. Pendry, J. B. et al. Magnetism from conductors and enhanced nonlinear phenomena. *IEEE Trans. Microwave Theory Tech.* 47, 2075 (1999).
- [160]. Smith, D. R. Composite medium with simultaneously negative permeability and permittivity. *Phys. Rev. Lett.* 84, 4184 (2000).
- [161]. Fang, N. et al. Sub-diffraction-limited optical imaging with a silver superlens. *Science* 308, 534 (2005).
- [162]. Zhao, Q. et al. Mie resonance-based dielectric metamaterials. *Materials today*, 12, 60 (2009).
- [163]. Yang, Y. Resonant All-Dielectric Optical Metamaterials. Doctoral dissertation, Vanderbilt University (2015).

- [164]. Kuznetsov, A. I. et al. Optically resonant dielectric nanostructures. *Science* 354, aag2472 (2016).
- [165]. Jahani, S. and Jacob, Z. All-dielectric metamaterials. *Nat. Nanotech.* 11, 23 (2016).
- [166]. Staude, I. and Schilling, J. Metamaterial-inspired silicon nanophotonics. *Nat. Photonics* 11, 274 (2017).
- [167]. Baranov, D. G. et al. All-dielectric nanophotonics: the quest for better materials and fabrication techniques. *Optica* 4, 814 (2017).
- [168]. Staude, I., Pertsch, T. & Kivshar, Y. S. All-dielectric resonant meta-optics lightens up. *ACS Photonics* 6, 802 (2019).
- [169]. Kruk, S. & Kivshar, Y. Functional meta-optics and nanophotonics governed by Mie resonances. *ACS Photonics* 4, 2638 (2017).
- [170]. Zhou, W. et al. Progress in 2D photonic crystal Fano resonance photonics. *Prog. Quant. Electron.* 38, 1 (2014).
- [171]. Khorasaninejad, M. & Capasso, F. Metalenses: Versatile multifunctional photonic components. *Science* 358, 8100 (2017).
- [172]. Lalanne, P. & Chavel, P. Metalenses at visible wavelengths: past, present, perspectives. *Laser & Photon. Rev.* 11, 1600295 (2017).
- [173]. Limonov, M. F. et al. Fano resonances in photonics. *Nat. Photonics* 11, 543 (2017).
- [174]. Shaltout, A. M. et al. Spatiotemporal light control with active metasurfaces. *Science* 364, eaat3100 (2019).
- [175]. Genevet, P. et al. Recent advances in planar optics: from plasmonic to dielectric metasurfaces. *Optica* 4, 139-152 (2017).
- [176]. Seyedeh, M. K. et al. A review of dielectric optical metasurfaces for wavefront control. *Nanophotonics* 7, 1041-1068 (2018).

- [177]. Yang, Y. M. et al. All-dielectric metasurface analogue of electromagnetically induced transparency. *Nat. Commun.* 5, 5753 (2014).
- [178]. Wu, C. et al. Spectrally selective chiral silicon metasurfaces based on infrared Fano resonances. *Nat. Commun.* 5, 3892 (2014).
- [179]. Miroshnichenko, A. E. et al. Nonradiating anapole modes in dielectric nanoparticles. *Nat. Commun.* 6, 8069 (2015).
- [180]. Yang, Y. M. et al. Nonlinear Fano-resonant dielectric metasurfaces. *Nano Lett.* 15, 7388-7393 (2015).
- [181]. Shen, Y. et al. Structural colors from Fano resonances. *ACS Photonics* 2, 27-32 (2015).
- [182]. Makarov, S. V. et al. Light-Induced tuning and reconfiguration of nanophotonic structures. *Laser & Photon. Rev.* 11, 1700108 (2017).
- [183]. Rybin, M. V. et al. High-Q supercavity modes in subwavelength dielectric resonators. *Phys. Rev. Lett.* 119, 243901 (2017).
- [184]. Gao, X. et al. Formation mechanism of guided resonances and bound states in the continuum in photonic crystal slabs. *Sci. Rep.* 6, 31908 (2016)
- [185]. Rybin, M. V. et al. Phase diagram for the transition from photonic crystals to dielectric metamaterials. *Nat. Commun.*, 6, 10102 (2015).
- [186]. Shipman, S. P. & Venakides, S. Resonant transmission near non-robust periodic slab modes. *Phys. Rev. E* 71, 026611 (2005).
- [187]. Yuan, L. & Lu, Y. Y. Bound states in the continuum on periodic structures: perturbation theory and robustness. *Opt. Lett.* 42, 4490 (2017).
- [188]. Sakoda, K. Symmetry, degeneracy, and uncoupled modes in two-dimensional photonic lattices. *Phys. Rev. B* 52, 7982 (1995).
- [189]. Hou, D. et al. D-band on-chip higher-order-mode dielectric-resonator antennas fed by half-mode cavity in CMOS technology. *IEEE Antennas Propag. Mag.* 56, 80 (2014)

- [190]. Friedrich, H. & Wintgen, D. Interfering resonances and bound states in the continuum. *Phys. Rev. A* 32, 3231 (1985).
- [191]. Poddubny, A. N. et al. Fano interference governs wave transport in disordered systems. *Nat. Commun.* 3, 914 (2012).
- [192]. Ma, Z. et al. Terahertz all-dielectric magnetic mirror metasurfaces. *ACS Photonics* 3, 1010 (2016).
- [193]. Al-Naib, I. et al. Effect of local field enhancement on the nonlinear terahertz response of a silicon-based metamaterial. *Phys. Rev. B* 88, 195203 (2013).
- [194]. Gu, J. et al. Active control of electromagnetically induced transparency analogue in terahertz metamaterials. *Nat. Commun.* 3, 1151 (2012).
- [195]. Zhang, S. et al. Photo-induced handedness switching in terahertz chiral metamolecules. *Nat. Commun.* 3, 942 (2012).
- [196]. Manjappa, M. et al. Active photo-switching of sharp Fano resonances in THz metadevices. *Adv. Mater.* 29, 1603355 (2017).
- [197]. Klimov, V. I. et al. Initial carrier relaxation dynamics in ion-implanted Si nanocrystals: Femtosecond transient absorption study. *Appl. Phys. Lett.* 73, 2603 (1998).
- [198]. Luk'yanchuk, B. et al. The Fano resonance in plasmonic nanostructures and metamaterials. *Nat. Mater.* 9, 707 (2010).
- [199]. Quaranta, G. et al. Recent advances in resonant waveguide gratings. *Laser & Photon. Rev.* 12, 1800017 (2018).
- [200]. Kintaka, K. et al. A guided-mode-selective focusing grating coupler. *IEEE Photon. Tech. Lett.* 16, 512 (2004).
- [201]. Homola, J. Surface plasmon resonance sensors for detection of chemical and biological species. *Chem. Rev.* 108, 462 (2008).

- [202]. Gongora, J. S. T. et al. Anapole nanolasers for mode-locking and ultrafast pulse generation. *Nat. Commun.* 8, 15535 (2017).
- [203]. Liu, S. et al. Resonantly enhanced second-harmonic generation using III–V semiconductor all-dielectric metasurfaces. *Nano Lett.* 16, 5426 (2016).
- [204]. Grinblat, G. et al. Enhanced third harmonic generation in single germanium nanodisks excited at the anapole mode. *Nano Lett.* 16, 4635 (2016).
- [205]. Shorokhov, A. S. et al. Multifold enhancement of third-harmonic generation in dielectric nanoparticles driven by magnetic Fano resonances. *Nano Lett.* 16, 4857 (2016).
- [206]. Shibamura, T. et al. Efficient third harmonic generation from metal–dielectric hybrid nanoantennas. *Nano Lett.* 17, 2647 (2017).
- [207]. Li, B. B. et al. Single nanoparticle detection using split-mode microcavity Raman lasers. *PNAS* 111, 14657 (2014).
- [208]. Brongersma, M. L. et al. Light management for photovoltaics using high-index nanostructures. *Nat. Mater.* 13, 451 (2014).
- [209]. Cong, L. et al. Fano resonances in terahertz metasurfaces: a figure of merit optimization. *Adv. Opt. Mater.* 3, 1537 (2015).
- [210]. Shyiq Amin, M. et al. Optical transmission filters with coexisting guided-mode resonance and Rayleigh anomaly. *Appl. Phys. Lett.* 103, 131106 (2013).
- [211]. Fehrembach, A. L. et al. 2×1 D crossed strongly modulated gratings for polarization independent tunable narrowband transmission filters. *JOSA A* 34, 234 (2017).
- [212]. Niraula, M. et al. Mode-coupling mechanisms of resonant transmission filters. *Opt. Express* 22, 25817 (2014).
- [213]. Niraula, M. et al. Concurrent spatial and spectral filtering by resonant nanogratings. *Opt. Express* 23, 23428 (2015).

- [214]. Khaleque, T. et al. Design and fabrication of broadband guided-mode resonant reflectors in TE polarization. *Opt. Express* 22, 12349 (2014).
- [215]. Mateus, C. F. et al. Ultrabroadband mirror using low-index cladded subwavelength grating. *IEEE Photon. Tech. Lett.* 16, 518 (2004).
- [216]. Ricciardi, A. et al. Broadband mirrors in the near-infrared based on subwavelength gratings in SOI. *IEEE Photon. J.* 2, 696 (2010).
- [217]. Khaleque, T. et al. Design and fabrication of broadband guided-mode resonant reflectors in TE polarization. *Opt. Express* 22, 12349 (2014).
- [218]. Magnusson, R. Wideband reflectors with zero-contrast gratings. *Opt. Lett.* 39, 4337 (2014).
- [219]. Yu, W. et al. Subwavelength grating wideband reflectors with tapered sidewall profile. *MRS Adv.* 1, 1683 (2016).
- [220]. Magnusson, R. Flat-top resonant reflectors with sharply delimited angular spectra: an application of the Rayleigh anomaly. *Opt. Lett.* 38, 989 (2013).
- [221]. Ko, Y. H. & Magnusson, R. Wideband dielectric metamaterial reflectors: Mie scattering or leaky Bloch mode resonance? *Optica*, 5, 289 (2018).
- [222]. Bark, H. S. et al. Transmission characteristics of all-dielectric guided-mode resonance filter in the THz region. *Sci. Rep.* 8, 13570 (2018).
- [223]. Ferraro, A. et al. Guided-mode resonant narrowband terahertz filtering by periodic metallic stripe and patch arrays on cyclo-olefin substrates. *Sci. Rep.* 8, 17272 (2018).
- [224]. Wang, S. S. & Magnusson, R. Theory and applications of guided-mode resonance filters. *Appl. Opt.* 32, 2606 (1993).
- [225]. Fano, U. The theory of anomalous diffraction gratings and of quasi-stationary waves on metallic surfaces (Sommerfeld's waves). *JOSA*, 31, 213 (1941).

- [226]. Liang, Y. et al. Three-dimensional coupled-wave model for square-lattice photonic crystal lasers with transverse electric polarization: A general approach. *Phys. Rev. B* 84, 195119 (2011).
- [227]. Peng, C. et al. Three-dimensional coupled-wave theory analysis of a centered-rectangular lattice photonic crystal laser with a transverse-electric-like mode. *Phys. Rev. B* 86, 035108 (2012).
- [228]. Peng, B. et al. What is and what is not electromagnetically induced transparency in whispering-gallery microcavities. *Nat. Commun.* 5, 5082 (2014).
- [229]. Lemarchand, F. et al. Study of the resonant behaviour of waveguide gratings: increasing the angular tolerance of guided-mode filters. *J. Opt. A: Pure and Appl. Opt.* 1, 545 (1999).
- [230]. Lepetit, T. et al. Resonance continuum coupling in high-permittivity dielectric metamaterials. *Phys. Rev. B* 82, 195307 (2010).
- [231]. Koshelev, K. et al. Asymmetric metasurfaces with high-Q resonances governed by bound states in the continuum. *Phys. Rev. Lett.* 121, 193903 (2018).
- [232]. Overvig, A. C. et al. Dimerized high contrast gratings. *Nanophotonics* 7, 1157 (2018).
- [233]. Nguyen, H. S. et al. Symmetry breaking in photonic crystals: On-demand dispersion from flatband to Dirac cones. *Phys. Rev. Lett.* 120, 066102 (2018).
- [234]. Wang, H. F. et al. Bound states in the continuum in a bilayer photonic crystal with TE-TM cross coupling. *Phys. Rev. B* 98, 214101 (2018).
- [235]. Kilic, O. et al. Controlling uncoupled resonances in photonic crystals through breaking the mirror symmetry. *Optics express*, 16, 13090 (2008).
- [236]. Overvig, A. C. et al. Selection rules for symmetry-protected bound states in the continuum. *arXiv preprint, arXiv:1903.11125* (2019).
- [237]. Jin, J. et al. Topologically enabled ultrahigh-Q guided resonances robust to out-of-plane scattering. *Nature* 574, 501 (2019).

- [238]. Schurig, D. et al. Metamaterial electromagnetic cloak at microwave frequencies. Science 314, 977 (2006).
- [239]. Cai, W. et al. Optical cloaking with metamaterials. Nat. Photonics 1, 224 (2007).
- [240]. Liu, R. et al. Broadband ground-plane cloak. Science 323, 366 (2009).
- [241]. Ziolkowski, R. W. Propagation in and scattering from a matched metamaterial having a zero index of refraction. Phys. Rev. E 70, 046608 (2004).
- [242]. Silveirinha, M. & Engheta, N. Design of matched zero-index metamaterials using nonmagnetic inclusions in epsilon-near-zero media. Phys. Rev. B 75, 075119 (2007).
- [243]. Huang, X. et al. Dirac cones induced by accidental degeneracy in photonic crystals and zero-refractive-index materials. Nat. Mater. 10, 582 (2011).
- [244]. Li, Y. et al. On-chip zero-index metamaterials. Nat. Photonics 9, 738 (2015).
- [245]. Liberal, I. & Engheta, N. Near-zero refractive index photonics. Nat. Photonics 11, 149 (2017).
- [246]. Vulis, D. I. et al. Manipulating the flow of light using Dirac-cone zero-index metamaterials. Rep. Prog. Phys. 82, 012001 (2018).
- [247]. Rotman, W. Plasma simulation by artificial dielectrics and parallel-plate media. IRE Trans. Antennas Propag. 10, 82 (1962).
- [248]. Vesseur, E. J. R. et al. Experimental verification of $n = 0$ structures for visible light. Phys. Rev. Lett. 110, 013902 (2013).
- [249]. Naik, G. V. et al. Oxides and nitrides as alternative plasmonic materials in the optical range. Opt. Mater. Express 1, 1090 (2011).
- [250]. Feigenbaum, E. et al. Unity-order index change in transparent conducting oxides at visible frequencies. Nano Lett. 10, 2111 (2010).
- [251]. Naik, G. V. et al. Alternative plasmonic materials: beyond gold and silver. Adv. Mater. 25, 3264 (2013).

- [252]. Pollard, R. J. et al. Optical nonlocalities and additional waves in epsilon-near-zero metamaterials. *Phys. Rev. Lett.* 102, 127405 (2009).
- [253]. Rizza, C. et al. Gain assisted nanocomposite multilayers with near zero permittivity modulus at visible frequencies. *Appl. Phys. Lett.* 99, 221107 (2011).
- [254]. Yun, S. et al. Low-loss impedance-matched optical metamaterials with zero-phase delay. *ACS Nano* 6, 4475 (2012).
- [255]. Maas, R. et al. Experimental realization of an epsilon-near-zero metamaterial at visible wavelengths. *Nat. Photonics* 7, 907 (2013).
- [256]. Yang, Y. et al. Terahertz topological photonics for on-chip communication. *arXiv preprint arXiv:1904.04213* (2019).
- [257]. Minkov, M. et al. Zero-index bound states in the continuum. *Phys. Rev. Lett.* 121, 263901 (2018).
- [258]. Sakoda, K. Proof of the universality of mode symmetries in creating photonic Dirac cones. *Opt. Express* 20, 25181 (2012).
- [259]. Wang, L. G. et al. Realization of Dirac point with double cones in optics. *Opt. Lett.* 34, 1510 (2009).