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## PAPER

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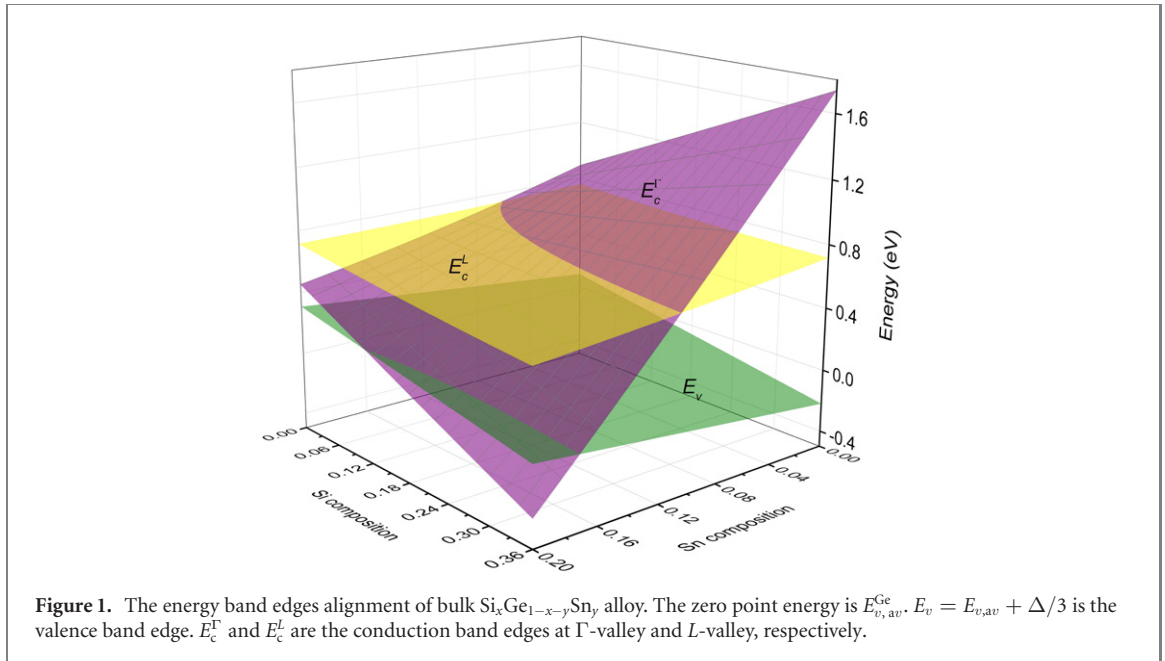
## Abstract

By carefully analyzing the latest composition-dependent parameters of SiGeSn alloys, we come to realize that this system could provide type-II energy band alignment at direct bandgap condition. The discovery inspires us to explore the mid-infrared interband cascade laser (ICL) in SiGeSn system. Based on the eight-band  $k \cdot p$  model, we theoretically design three schemes of ICL, in which the active region and the carrier injectors are optimized simultaneously. Afterward, the properties of TE-mode optical gain spectrums and differential gain are investigated individually for each scheme. Furthermore, the spontaneous emission spectrums and radiative current density are also calculated. Our theoretical results indicate that the active region composed of double-electron and triple-hole quantum wells has the best gain performance, reaching  $660 \text{ cm}^{-1}$  for a single period of the ICL under  $7.8 \times 10^{18} \text{ cm}^{-3}$  injected electron density. This work opens up another type of infrared lasers that can be developed from the group-IV system, offering a new pathway to achieving the monolithic integration in Si photonics.

## 1. Introduction

Driven by the mature microelectronics industry, the CMOS-compatible silicon photonics, providing the possibility of monolithic optoelectronics integration, has been long pursued since 1990s [1–3]. Despite the great progress in Si-based waveguides, photodetectors and modulators, the inherent indirect-bandgap property of the elemental semiconductors Si and Ge has prevented them from being utilized for the development of efficient light emitters. Exploring efficient group-IV light sources has become a fundamental and challenging task for silicon photonics community. Since the unstrained GeSn alloy is observed to become a direct-bandgap semiconductor when Sn concentration exceeds about 8% [4, 5], the novel group-IV materials such as binary GeSn and ternary SiGeSn alloys have attracted great attention. In recent years, optically pumped lasing has been demonstrated by several groups from these group-IV alloys [6–11]. Compared to the type-I aligned bulk GeSn/SiGeSn heterostructure, the multiple quantum well (QW) structure could sharply lower the lasing threshold [12] as predicted in an earlier study [13]. All these progress have stimulated the exploration of electrically pumped lasers in group-IV system.

Besides the above-mentioned traditional interband laser, many efforts have also been devoted to the research of quantum cascade laser (QCL) in SiGe system [14–22]. Compared to the conduction band offset (CBO), the relatively larger valence band offset (VBO) prompted investigation of QCL schemes based on transitions between valence subbands [18], inspired by an early proposal [23]. Some other designs utilizing conduction subbands at  $\Delta$ -valley [19] and  $L$ -valley [17] have also been proposed. Similar to QCLs, interband cascade laser (ICL) involving the recombination between electrons and holes offers a different kind of cascade configuration. Owing to the relatively longer upper-state carrier lifetime and voltage-efficient cascade scheme, ICL possesses higher quantum efficiency and lower threshold power density in comparison with QCLs. In fact, ICL has been widely investigated and show great potentials in



mid-infrared applications such as trace gas sensing, industrial process control and free-space optical communication [24–26]. However, to our best knowledge, the work on ICLs so far is only focused on InAs/GaSb system because of their type-II band alignment requirement. It is natural to raise a question: is it possible to realize ICL in group-IV system?

In this work, we theoretically investigate the possibility of ICL configurations in group-IV system. The eight-band  $k \cdot p$  theory is utilized to design three specific ICL schemes based on the SiGeSn system. In order to facilitate the experimental community to take the designs as references, we have calculated the wavefunctions and energy levels associated with active region, electron and hole injectors. Furthermore, optical gain spectrums under different injection conditions and corresponding differential gain are investigated for the three schemes individually. Finally, because the spontaneous emission and radiative current density have a significant impact on the laser performance, we have studied their dependence on the different injection conditions. Our results confirm the feasibility of implementing ICLs in SiGeSn system and the gain coefficient of single period can reach  $660 \text{ cm}^{-1}$  under  $7.8 \times 10^{18} \text{ cm}^{-3}$  injected carrier density.

## 2. Theoretical model

In group-IV system, Ge is an indirect-bandgap semiconductor whose conduction band minimum locates at  $L$ -valley, only 135 meV lower than  $\Gamma$ -valley. Sn atoms are commonly used to partially replace Ge atoms in GeSn alloy to lower down the conduction band at  $\Gamma$ -valley. With the increase of Sn concentration, GeSn alloy has the opportunity to become a direct-bandgap semiconductor that can be used for light source. For the multiple QW and superlattice based optoelectronic devices in group-IV system, Si can also be incorporated to increase the diversity of band alignment. The key parameter  $E_{v,av}$  of  $\text{Si}_x\text{Ge}_{1-x-y}\text{Sn}_y$  ternary alloy, namely the averaged band offsets, can be written as

$$E_{v,av}(x, y) = (1 - x - y)E_{v,av}^{\text{Ge}} + xE_{v,av}^{\text{Si}} + yE_{v,av}^{\text{Sn}}. \quad (1)$$

The parameters in equation (1) are adopted from reference [27], in which the  $E_{v,av}$  are in best agreement with existing experimental data and/or *ab initio* theoretical calculations. Besides the averaged band offsets, the bandgap of  $\text{Si}_x\text{Ge}_{1-x-y}\text{Sn}_y$  alloy is another important parameter that does not strictly obey the Vegard's law. Generally, the compositional dependence of bandgap can be described by introducing the bowing effect [27],

$$E_t(x, y) = E_t^{\text{Ge}}(1 - x - y) + E_t^{\text{Si}}x + E_t^{\text{Sn}}y - b^{\text{GeSi}}(1 - x - y)x - b^{\text{GeSn}}(1 - x - y)y - b^{\text{SiSn}}xy, \quad (2)$$

where  $t = \Gamma, L$ . As shown by equation (2), the quadratic compositional dependence is represented by the bowing coefficients  $b$ , whose values are adopted from reference [28] except  $b_{\Gamma}^{\text{SiSn}}$ . The determination of  $b_{\Gamma}^{\text{SiSn}}$

**Table 1.** The main parameters of bulk Si, Ge and Sn at 300 K [27, 28]. The energy parameters are in eV and the lattice constant is in Å.

	$E_{v,av}$	$\Delta$	$E_g^\Gamma$	$E_g^L$	$m_c$	$\gamma_1$	$\gamma_2$	$\gamma_3$	$a_c^\Gamma$	$a_v$	$b_v$	$a_0$
Si	-0.8	0.044	4.185	1.65	0.528	4.22	0.39	1.44	1.98	2.46	-2.1	5.4307
Ge	0.0	0.29	0.7985	0.664	0.038	13.38	4.24	5.69	-8.24	1.24	-2.9	5.6573
Sn	0.904	0.8	-0.413	0.092	-0.058	-15.0	-11.45	-8.55	-5.33	1.55	-2.7	6.4892

value is challenging, owing to the lattice mismatch would lower down the quality of SiSn alloys that hinders the measurement. In 2016, Wendav *et al* reported a much larger  $b_\Gamma^{\text{SiSn}}$  value ( $=24$  eV) determined by photoluminescence experimentally [29], until last year Menendez *et al* obtained a similar result ( $=25.6$  eV) by electroluminescence experimentally [27]. These researches confirmed the large bowing effect induced by the SiSn component. In this work, we refer to the updated parameters to design the band alignment. Taking the parameters from references [27, 28], figure 1 is plotted to display the energy band edges of bulk SiGeSn ternary alloys. As shown in figure 1, with the increase of Sn and Si compositions,  $E_c^\Gamma$  will be lower than  $E_c^L$ , which indicates the transition into a direct-bandgap semiconductor. Noticing that  $E_v$  is an inclined plane with the variation of alloy composition, there is a room near the intersecting lines between  $E_c^\Gamma$  and  $E_v$  to pick out the type-II broken-gap alignment at direct bandgap condition.

Whereafter, the envelope-function theory based on eight-band  $k \cdot p$  model is utilized to design the band structures and wavefunctions of the ICL at  $\Gamma$ -valley. Since the SiGeSn alloy still holds the diamond crystal structure, the Hamiltonian used here is based on the Burt–Foreman theory, which takes account of the boundary conditions for superlattice [30]. The Pikus–Bir strain Hamiltonian is also incorporated as the way described in [31]. The total Hamiltonian can be written as

$$H = \begin{pmatrix} E_c + A & 0 & -\sqrt{3}v & \sqrt{2}u & v^\dagger & 0 & u & \sqrt{2}v^\dagger \\ 0 & E_c + A & 0 & -v & \sqrt{2}u & \sqrt{3}v^\dagger & \sqrt{2}v & -u \\ -\sqrt{3}v^\dagger & 0 & -P - Q & S_- & -R & 0 & \frac{S_-}{\sqrt{2}} & -\sqrt{2}R \\ \sqrt{2}u^\dagger & -v^\dagger & S_-^\dagger & -P + Q & -C & -R & \sqrt{2}Q & -\sqrt{\frac{3}{2}}\Sigma_- \\ v & \sqrt{2}u^\dagger & -R^\dagger & -C^\dagger & -P + Q & -S_+^\dagger & -\sqrt{\frac{3}{2}}\Sigma_+ & -\sqrt{2}Q \\ 0 & \sqrt{3}v & 0 & -R^\dagger & -S_+ & -P - Q & \sqrt{2}R^\dagger & \frac{S_+}{\sqrt{2}} \\ u^\dagger & \sqrt{2}v^\dagger & \frac{S_-^\dagger}{\sqrt{2}} & \sqrt{2}Q^\dagger & -\sqrt{\frac{3}{2}}\Sigma_+^\dagger & \sqrt{2}R & -P - \Delta & -C \\ \sqrt{2}v & -u^\dagger & -\sqrt{2}R^\dagger & -\sqrt{\frac{3}{2}}\Sigma_-^\dagger & -\sqrt{2}Q^\dagger & \frac{S_+^\dagger}{\sqrt{2}} & -C^\dagger & -P - \Delta \end{pmatrix} \quad (3)$$

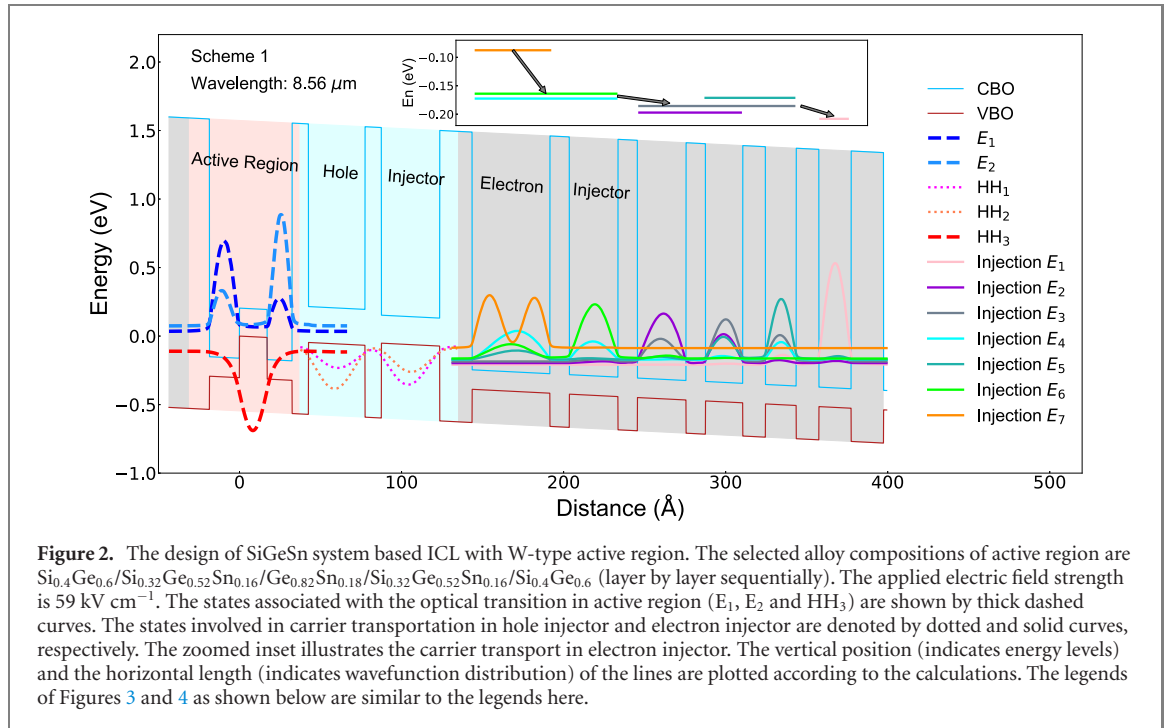
where the details of each term in equation (3) can be found in references [32–34]. The bulk material parameters used for calculations are listed in table 1. All the calculations in this work are performed at 300 K. The numerical solutions are obtained by the plane-wave expansion method [28, 35].

Afterward, the TE-mode interband gain spectrums can be investigated under different injection conditions. For semiconductor lasers, the optical gain spectrum and spontaneous emission spectrum can be written as [36]

$$g(\hbar\omega) = \frac{\pi e^2}{n_r c \epsilon_0 m_0^2 \omega} \sum_{m,n} \int_0^\infty \rho^{2D} M_{m,n} (f_c^m - f_v^n) \mathcal{L}(\hbar\omega) dE_t, \quad (4)$$

$$R_{sp}(\hbar\omega) = \frac{\omega n_r e^2}{\pi c^3 \hbar \epsilon_0 m_0^2} \sum_{m,n} \int_0^\infty \rho^{2D} M_{m,n} f_c^m (1 - f_v^n) \mathcal{L}(\hbar\omega) dE_t, \quad (5)$$

where  $\mathcal{L}(\hbar\omega) = \text{sech}\left(\frac{E_{mm} + E_t - \hbar\omega}{\gamma}\right) / \gamma \pi$  is the broadening function which is more realistic than the Lorentzian lineshape [37].  $\rho^{2D}$  is the two-dimensional density of state estimated by the parabolic energy band dispersion,  $M_{m,n} = |\langle \psi_{cm} | \mathbf{e} \cdot \mathbf{p} | \psi_{vn} \rangle|^2$  is the momentum matrix element (MME) between the  $m$ th electron and the  $n$ th hole states.  $f_c^m$  and  $f_v^n$  are the Fermi–Dirac distribution for electrons and holes with quasi-Fermi levels  $E_{f(c,v)}$ , whose values are related to the carrier density and operating voltage.  $2\gamma$  is the spectrum broadening factor, which is chosen to be 30 meV here. At last, the differential gain and radiative current density  $J_{rad}$  can be calculated by  $\frac{dg}{dn}$  and  $J_{rad} = qL_z \int_0^\infty R_{sp}(\hbar\omega) d(\hbar\omega)$ , respectively.



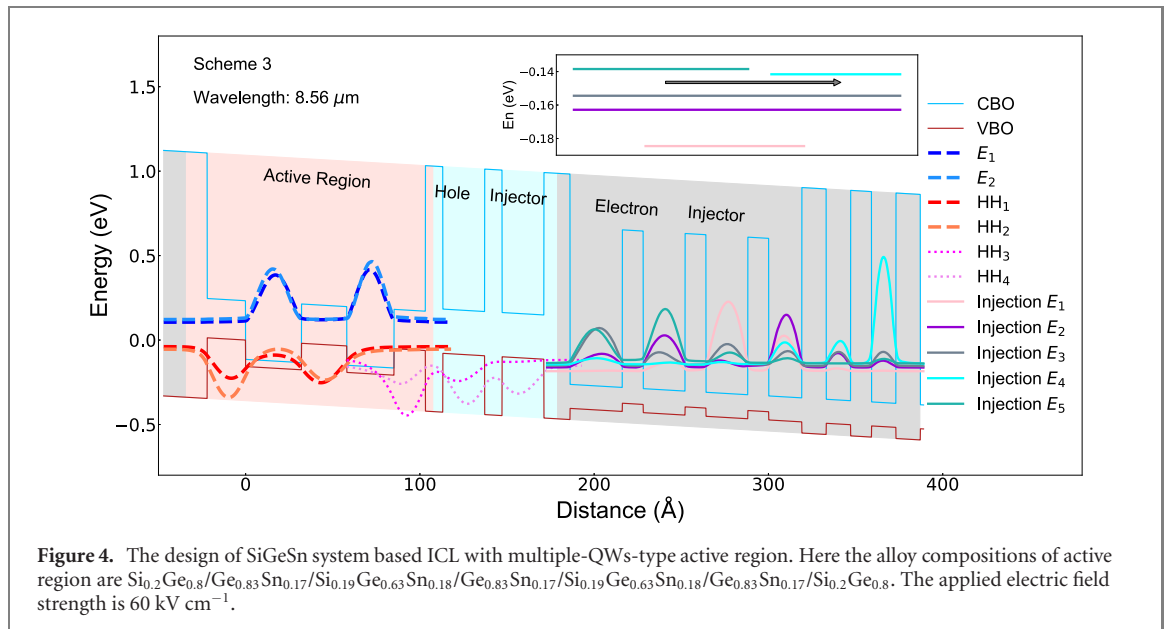
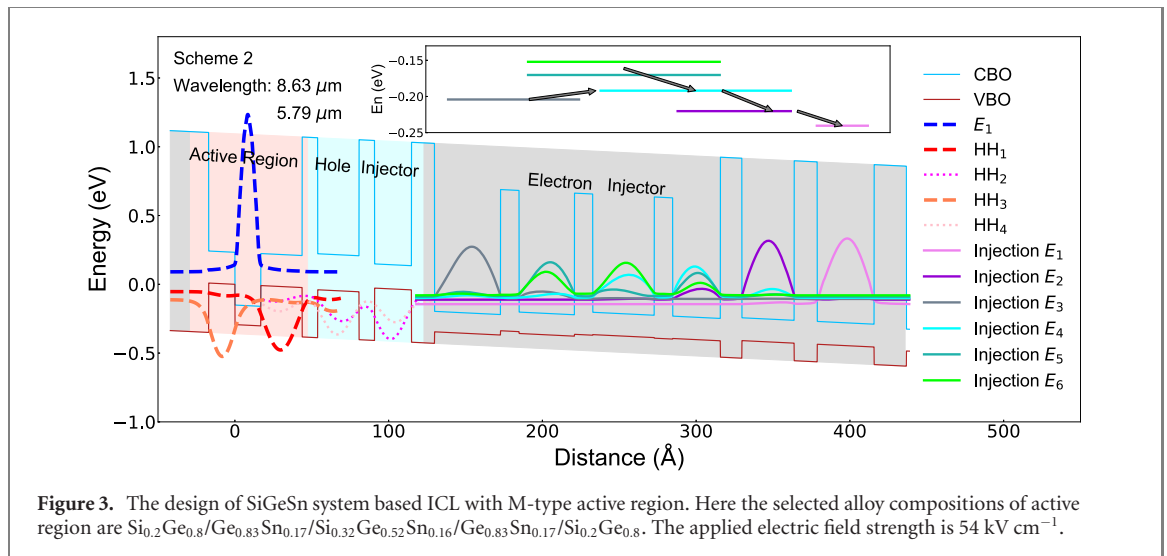
### 3. Results and discussion

For ICL based on InAs/GaSb system, the W-type active region with two InAs electron QWs and one InGaSb hole QW has become a standard feature of the state-of-the-art ICL design and shown good performance experimentally. Hence, we inherit the basic concept there as the starting point and propose three types of ICL in SiGeSn system. In our design, the entire period of ICL including active region, electron and hole injectors are calculated simultaneously, from the viewpoint of practicability. All the three schemes are designed to emit at around  $8.6 \mu\text{m}$  for easy comparison. As shown in figure 2, two electron QWs and one hole QW construct the W-type active region of the first scheme. The first and second electron ( $E_1$  and  $E_2$ ) wavefunctions both have the double-peaked shape due to the active region configuration. The third heavy-hole ( $\text{HH}_3$ ) wavefunction is enclosed by the two ground state electron wavefunctions. The injected electrons recombine with holes in the active region and continue to flow into the injectors. The first and second heavy-hole ( $\text{HH}_1$  and  $\text{HH}_2$ ) are designed to reside in the hole injector and facilitate to the carrier transport. Specially, the  $\text{HH}_1$  and  $\text{HH}_2$  energy levels are carefully aligned to the most left  $E_7$  energy level in electron injector for transport consideration. Meanwhile, the electron wavefunctions and energy levels in the electron injector are deliberately aligned as a staircase. The electron injector with multiple QWs design can provide the tunability of electron states, which guarantees the efficient carrier injection to the next period.

In contrary to the first design, the second scheme with the M-type active region composed of one electron QW and two hole QWs is proposed and shown in figure 3. Unlike the double-peaked electron wavefunctions in scheme one, here the wavefunctions of  $\text{HH}_1$  and  $\text{HH}_3$  labeled by the red and coral dashed curves are single-peaked and both contribute to the optical transition. Meanwhile, the  $\text{HH}_2$  and  $\text{HH}_4$  states denoted by the dotted curves in the hole injector couple the carriers in active region and in electron injector. The states in electron injector are also optimized for transport.

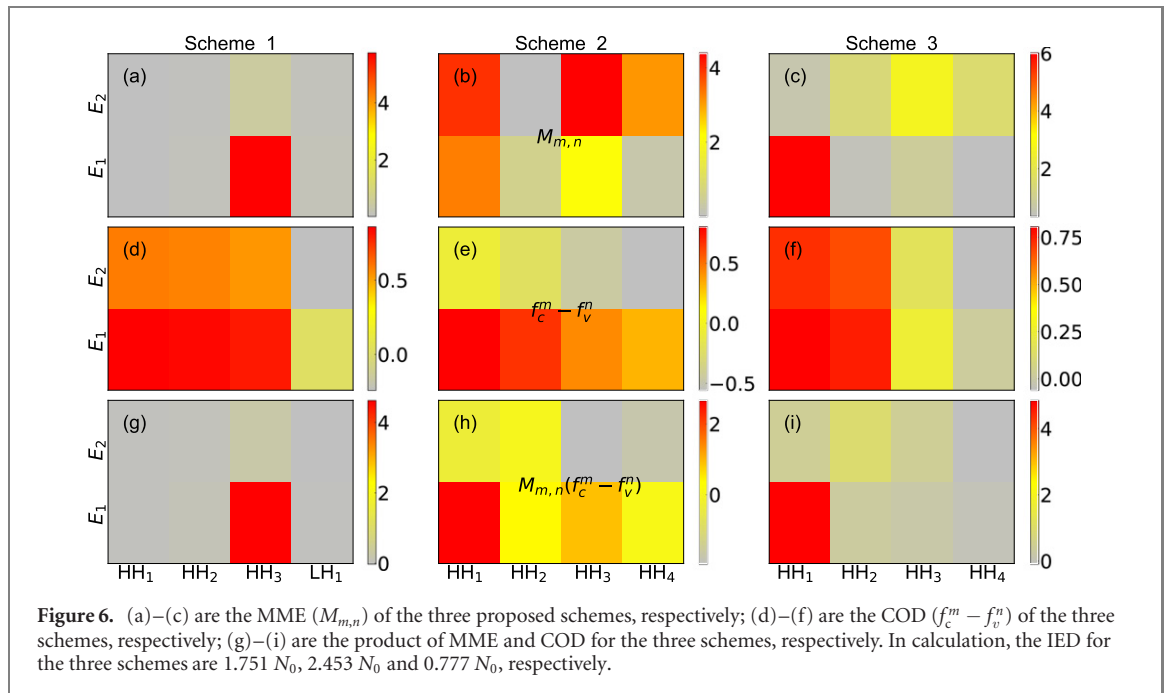
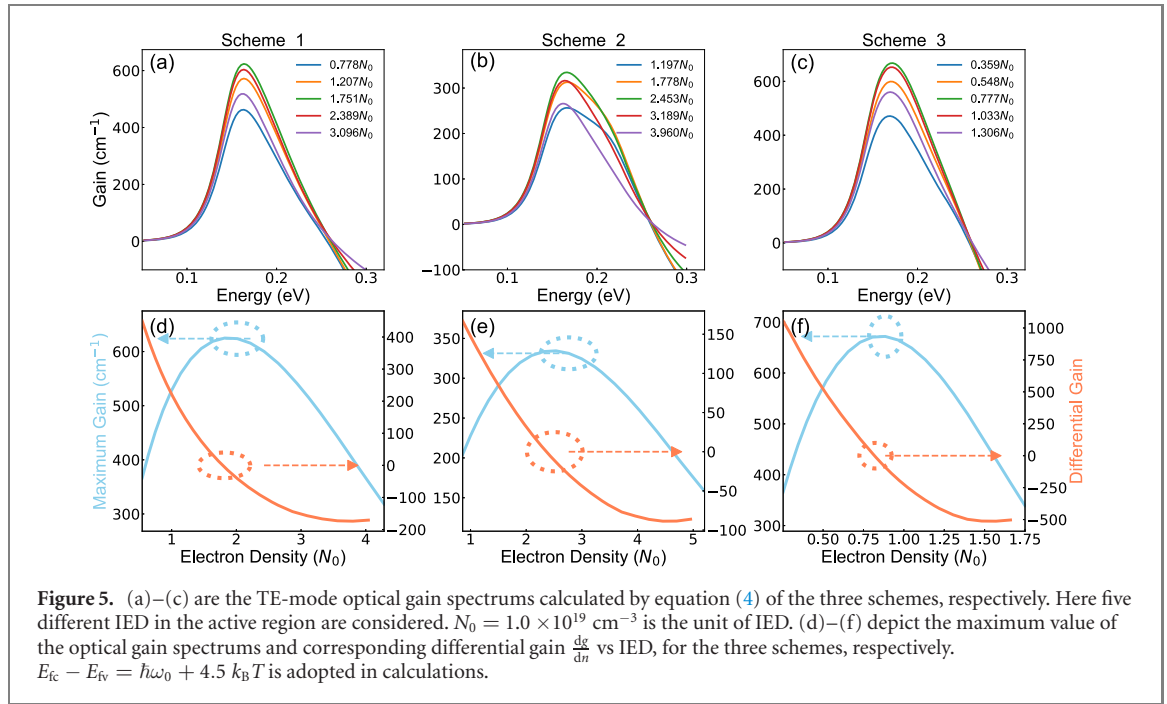
Enlighten by the above-proposed schemes, naturally the third design can be regarded as a combination: the active region contains two electron QWs and three hole QWs. To realize the double-peaked hole wavefunctions, the alloy composition of electron QWs has been refined to form a lower energy barrier for the hole states in active region. As a result, all of the first two electron and hole wavefunctions have the double-peaked shape as shown in figure 4. Here the design principle of injectors is similar to the above two schemes.

After demonstration of the specific energy states and wavefunctions for the proposed ICL schemes, the important optical gain properties are to be investigated here. Figures 5(a)–(c) illustrate the TE-mode optical gain spectrums of the three schemes under different injected electron density (IED), respectively. In calculations, the same quasi-Fermi level separation ( $E_{fc} - E_{fv}$ ) is adopted for the three schemes for a straightforward comparison. At a rough glance, schemes 1 and 3 show the similar single-peaked gain



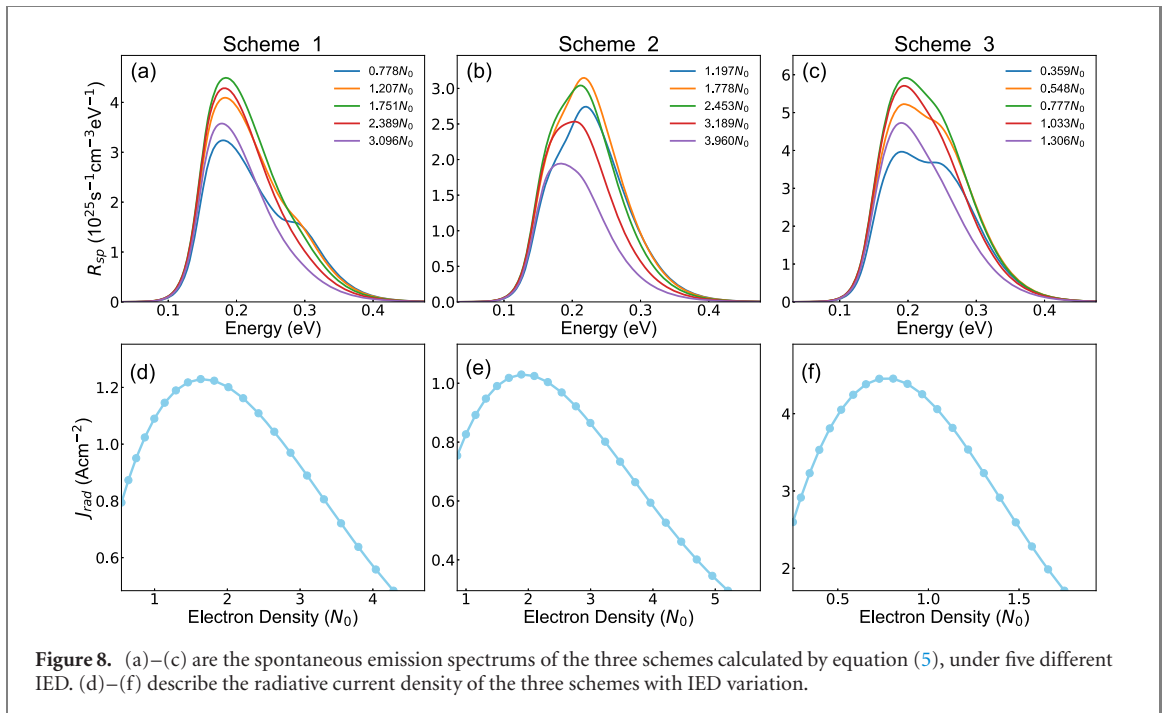
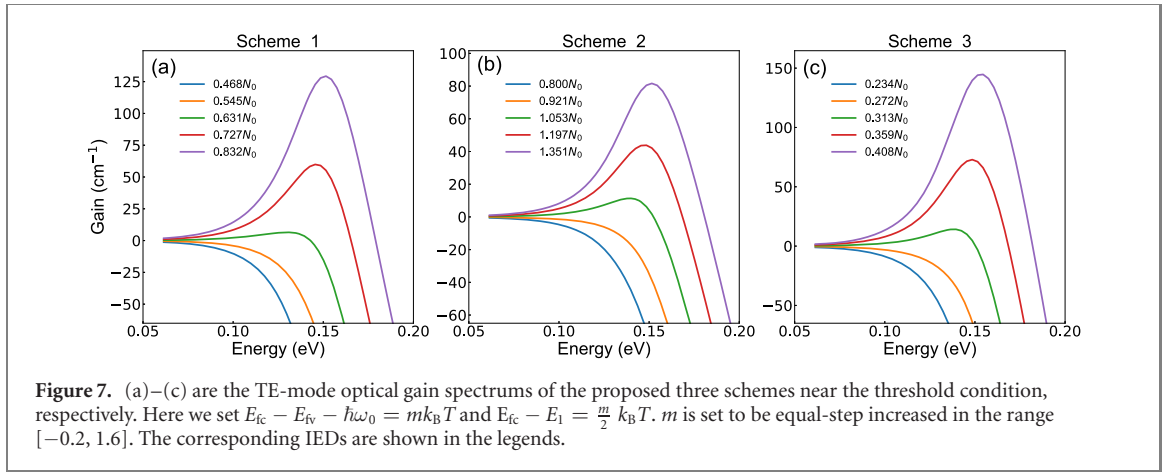
spectrum profile, whereas the gain spectrum profile of scheme 2 possesses the broadband characteristic. The distinct gain profile difference can be explained by the much different quantum transition characteristics of the three schemes. Let us decompose the gain spectrum formula described by equation (4) to find the reason. MME and carrier occupation difference (COD) play essential roles in gain profile generation. Therefore, we calculate the MME, COD and their product at zero wavevector for the three schemes, individually. As demonstrated in figure 6, the MME and COD cannot always reach maximum at the same optical transition. Taking scheme 2 for example, the  $E_1\text{--}HH_{1,3}$  and  $E_2\text{--}HH_{1,3,4}$  transitions all have considerable MME strength. However, considering the carrier occupation aspect, the  $E_2\text{--}HH_{1,3,4}$  transitions are much more ineffective than the others. Hence these three transitions hardly contribute to the overall optical gain spectrum, as indicated in figure 6(h). As a result, the  $E_1\text{--}HH_1$  and  $E_1\text{--}HH_3$  transitions construct the main gain profile of scheme 2,  $E_1\text{--}HH_2$  transition does a small contribution as well. The similar analysis can be performed to scheme 1 and 3 as well. As a result, we determine that the  $E_1\text{--}HH_3$  transition leads to the gain profile of scheme 1; the  $E_1\text{--}HH_1$  transition forms the main gain profile of scheme 3, other transitions merely contribute to the small gain profile broadening on the right-side.

Now let us investigate the gain spectrum evolution with the IED variation. As shown in figures 5(a)–(c), with the gradual increase of electron density, the gain spectrum intensity of all the three schemes experience an increase and then a decrease. In order to get a deeper insight into this phenomenon, we calculate the variation of maximum gain and differential gain with the increase of IED, as displayed in figures 5(d)–(f). Apparently, the maximum gain curves of all the three schemes show a concave shape plotted by the light blue lines, accompanied with the differential gain curves go across the zero point plotted by the coral lines.



It indicates there exists an inflection point for the maximum gain curve. The critical electron density can be extracted from the differential gain curve by setting the differential gain value to zero, as depicted by the coral dash circles in figures 5(d)–(f). The critical point gives out the optimal IED, beyond which the optical gain intensity would start to drop down. The occurrence of inflection point can be explained by the electron and hole occupation states. For the bipolar lasers such as ICL, actually the amount of effective electron–hole pairs in the active region determines the optical gain intensity. When the ICL is working,  $E_{fc} - E_{fv} = qFL$  is established under quasi-equilibrium condition, where  $F$  and  $L$  are the electric field strength and one period length respectively [26]. In the situation here,  $E_{fc}$  would be lifted up by the increased electron density in the active region, consequently  $E_{fv}$  would also be moved toward the conduction band direction due to keep a constant quasi-Fermi level separation. If  $E_{fv}$  is far beyond the hole energy levels in the active region, there would be no enough holes provided for the radiative recombination. Therefore, the inflection point phenomenon of the optical gain occurs here.

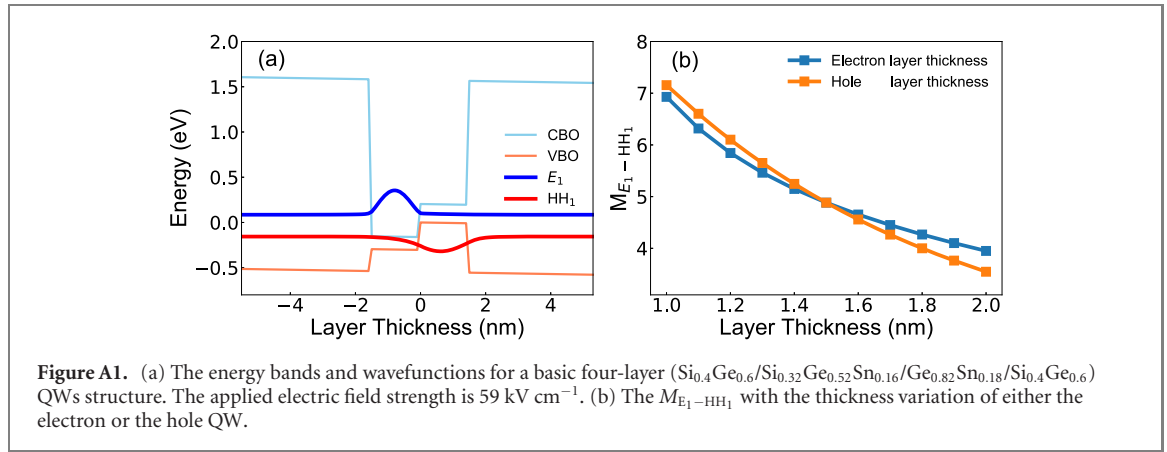
Comparing the optical gain spectra of the three proposed schemes, it is obvious that scheme 3 possesses the strongest gain intensity per IED investigated. Specifically, the maximum gain of scheme 3 can



reach  $660 \text{ cm}^{-1}$  under  $0.78 \times 10^{19} \text{ cm}^{-3}$  IED; whereas, to reach a similar level of maximum gain, scheme 1 needs  $1.75 \times 10^{19} \text{ cm}^{-3}$  IED; scheme 2 does not have the ability to do so. On the other hand, by further optimizing different transitions induced optical gain, scheme 2 provides the possibility to realize the flat broadband gain profile and then benefits to the exploration of optical frequency comb in SiGeSn system. Besides, scheme 2 could be used as the dual-wavelength laser by further separating the optical transitions in gain profile.

In addition, the TE-mode optical gain spectrums of the three schemes under lower carrier density are also investigated. Here we set  $E_{fc} - E_{fv} < \hbar\omega_0$  as the starting point, then we equally move the quasi-Fermi levels toward the opposite direction to gradually increase the energy separation until the optical gain occurs. As shown in figure 7, all the lowest-energy transitions for the three schemes evolve from absorption to gain with the increased IED. Whereas the higher energy transitions have the absorption characteristic. The reason is the quasi-Fermi level separation provides the capability of optical gain [36], here the adopted maximum separation is only  $\hbar\omega_0 + 1.6k_B T$ , which cannot drive enough optical gain of the higher energy transitions. The transparency electron densities are extracted from figure 7 as well, the values are about  $0.631, 1.053$  and  $0.313 \times 10^{19} \text{ cm}^{-3}$  for the three schemes, respectively. For a more realistic consideration, assuming the ICL is fabricated into a 3 mm long Fabry–Perot waveguide, the threshold material gain for a seven-stage ICL is roughly estimated to be  $55 \text{ cm}^{-1}$ , under the assumption that the total optical confinement is about 0.3 [13], the effective refractive index is about 4 and the cavity loss is about  $13 \text{ cm}^{-1}$ .

At last, the spontaneous emission spectrums and radiative current density corresponding to figure 5's injection condition are investigated. As shown in figure 8(a)–(c), the spontaneous emission spectrums



always keep the positive values. Scheme 1 is able to show the shoulder like profile, whereas the spectrums of scheme 3 show the slightly broadband characteristic. Schemes 1 and 2 have a smaller radiative current density than scheme 3, which may mean the lower power consumption from engineering viewpoint. Furthermore, the radiative current density of the three schemes also present the inflection point phenomenon with IED variation, which could provide guidance for practical design as well. The characteristics of spontaneous emission spectrums and radiative current density can be explained in a similar method as that for the gain spectrums, but not expanded here.

Although three designs of ICL based on SiGeSn system are proposed in this work, it still takes great effort to realize the ICL experimentally. The main concern is the challenging material growth tricks of SiGeSn alloys. With the endeavor of material scientists, GeSn alloy with Sn composition up to 33% has been synthesized by the chemical vapor deposition technique recently [38]. The progress in the material growth of SiGeSn alloys, could speed up the development of group-IV based devices. For the theoretical aspect, a more complicated 30-band  $k \cdot p$  method can be developed to explore the inter-valley transfer problems in SiGeSn based low-dimensional structures [39]. The more precise transport model based on non-equilibrium Green's function and density matrix theories are also required to be explored for the SiGeSn based ICL [21, 40].

#### 4. Conclusion

In summary, we propose three mid-infrared ICL designs in SiGeSn system and theoretically analyze their lasing feasibility based on a type-II band alignment that can be achieved with SiGeSn alloys in direct bandgap condition. The active region with double-electron and triple-hole QWs shows the best optical gain performance. The M-type active region has the possibility to become the platform for optical frequency comb. The optical gain and spontaneous emission of the proposed schemes exhibit distinct spectral profiles. Furthermore, the maximum gain spectrum and radiative current density show the inflection point phenomenon. Our design work brings forward a new kind of lasers that can be explored and potentially implemented monolithically in silicon photonics.

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#### Appendix A

As a supplement, we calculate the momentum matrix element between  $E_1$  and  $HH_1$  states ( $M_{E_1-HH_1}$ ) of a basic type-II interface structure in SiGeSn system. As shown in figure A1(a), the single electron and hole QWs surrounded by two barriers on both sides construct the four-layer structure. By changing the thickness of either of the two QWs, as demonstrated in figure A1(b), the momentum matrix elements increase monotonously with the decrease of QW thickness.

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