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Effect of temperature and thickness of graphene on the hydrogen storage properties

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Abstract

Hydrogen, of which the application is limited due to the difficulties in finding the ideal storage material, has been considered alternative for petroleum as the main energy source. With its large surface area and other extraordinary physical properties, graphene has been the focus of many researchers as the promising candidate for hydrogen storage and transportation. In this work, the hydrogen storage characteristics of graphene have been investigated by MD simulations. We found that, under the temperature of 70 K and the pressure of 1 MPa, the hydrogen uptake percentage can be as high as 54%. And the majority of the hydrogen atoms are absorbed during the initial 100–200 ps of the simulation. Moreover, the hydrogen storage properties of graphene with different environment temperatures have been studied. We found that with increasing temperature, the hydrogen uptake percentage towards the end of the simulation decreases. Furthermore, the number of layers of the graphene sheet also exerts influence of the hydrogen absorption capability of the sample. We conclude that the more graphene sheets are being used, the less hydrogen atoms are being absorbed by the sample. Our work provides insight into optimizing the environmental temperature and thickness of the graphene sheet when designing novel energy storage devices, especially hydrogen storage devices.

Introduction

Fossil fuel, such as petroleum, is one of the most commonly used energy source. However, the concern over its sustainability and the environmental issues resulting from excessive usage of petroleum lead to extensive discussions of finding an alternative for petroleum. Hydrogen has long been considered as one of the candidates because of its benign combustion products [1-4]. However, the application of hydrogen as an energy source commercially has been limited due to the difficulties of finding appropriate storage material for it [5]. Both graphene and CNT has also been used as a material for hydrogen storage [6-11]. In this work, comprehensive molecular dynamics simulations have been carried out to study the hydrogen absorption capacity of graphene. Specifically, the percentages of hydrogen absorbed by the graphene sample have been studied. Additionally, the temperature effect on the absorption is studied from 70 K to 300 K. Last but not least, the effect of the thickness of the graphene is also investigated.

Simulation Method

The MD simulations were performed using LAMMPS [12], which is a classical molecular dynamics code, and an acronym from large-scale atomic/molecular massively parallel simulator. The adaptive intermolecular reactive bond order (AIREBO [13]) potential was adopted. The potential allows for covalent bond breaking and forming, which enables accurate description of interactions between bonds. The simulations are performed using canonical ensemble with constant number of particles, volume and temperature. The time step is 0.1 fs.

To study the hydrogen absorption of a typical graphene, a single layer of graphene, which contains 1008 carbon atoms, is simulated. And it is positioned in the hydrogen reservoir, as shown in Figure 1. The graphene sample is fixed and the system is relaxed to observe the hydrogen absorption process. And the number of hydrogen atoms in the system is decided by the van der Waals equation of state under pressure of 1 MPa and at temperature of 70 K [14]. Temperature effects from 70 K to 300 K were studied. The effect of the thickness of the graphene on the hydrogen absorption is investigated by increasing the number of layers of graphene sample from 1 to 5.

Figure 1: System configuration of one single layer graphene positioned in the hydrogen reservoir. Red atoms represent carbon atoms and blue atoms represent hydrogen atoms.

Results and Discussions

To study the hydrogen storage properties of a single layer graphene sheet, the hydrogen uptake percentage is plotted as a function of time in Figure 2. It can be observed from the curve that about 54% of hydrogen atoms of the system are absorbed by the graphene at the initial 200 ps. Beyond that point, further relaxation of the system leads to fluctuation of the hydrogen uptake percentage around 54%. The high hydrogen absorption rate is the result of the exposure of both sides of the

single layer graphene in the hydrogen environment. Initially, when there are few hydrogen atoms in the sample, most of the hydrogen atoms rushed into the CNS. The process is slowed down by the increasing number of hydrogen on the graphene sample. And after all the available locations on the graphene are occupied by attached hydrogen, the capacity of graphene has reached a plateau state, where further increase of hydrogen absorption is unstable.

Figure 2: Hydrogen uptake percentage plotted as a function of time.

The effect of temperature on the hydrogen absorption of single layer graphene is studied by altering the temperature of the system from 70 K to 300 K. The results under various temperatures have been plotted and are shown in Figure 3. It is obvious from the curve that the hydrogen uptake percentage of the single layer graphene is decreasing with the increase of temperature. Under the temperatures of 70 K and 100 K, more than 40% of the hydrogen atoms are found to attach to both sides of the graphene. With the temperature higher than 200 K, less than 10% of the hydrogen atoms can be absorbed. This decreasing trend can be explained by the more rapid free movements of the hydrogen atoms under higher temperature. Specifically, under higher temperature, the movements of hydrogen atoms are higher. Therefore, it is harder for the single layer graphene to absorb the hydrogen atoms.

Figure 3: The variation of hydrogen uptake percentage of single layer graphene sheet after the system reaches the plateau statues with different temperature.

To study the effect of layering on the hydrogen uptake percentage of graphene, various layers of graphene sheets have been stacked up in the system. The total hydrogen uptake percentage of the graphene samples have been plotted as a function of time and shown in Figure 4. Similar trends can be observed from each of the five cases. In other words, the majority of the hydrogen atoms were absorbed at the initial stage from 0 ps to 200 ps. And beyond that point, negligible number of hydrogen atoms is absorbed. Moreover, the percentage of hydrogen atoms attached to the graphene sample throughout the simulation is decreasing with the increase in the thickness of the graphene. With more layers, the sample absorbed fewer hydrogen atoms. To further investigate of the effect of layering, the system has been sectioned into different number of layers according to the thickness of the graphene sample (of which the schematic figure is shown in Figure 5 and the distribution of the hydrogen atoms are plotted and shown from Figures 6 to 9. One obvious trend can be observed from each of the figure is that the interlayer area of graphene sample contains negligible number of hydrogen atoms. And majority of the hydrogen atoms attached are found on the top and bottom side of the sample. Therefore, it is reasonable to conclude that when being positioned into hydrogen reservoir, the multi-layer graphene samples absorbed hydrogen atoms mainly on the outer periphery.

Figure 4: The hydrogen uptake percentage of graphene with various thickness under the temperature of 70 K as a function of time.

Figure 5: The schematic figure of how the multi-layer graphene sheets are divided. The top section (section 1) is defined from the center of the first layer of graphene to the top with a height of 3.4 Å. Similar approach is used to define the bottom section (section 6).

Figure 6: The distribution of the attached hydrogen atoms as a function of time in the case of two layers graphene sample.

Figure 7: The distribution of the attached hydrogen atoms as a function of time in the case of three layers graphene sample.

Figure 8: The distribution of the attached hydrogen atoms as a function of time in the case of four layers graphene sample.

Figure 9: The distribution of the attached hydrogen atoms as a function of time in the case of five layers graphene sample.

Conclusion

In this work, the hydrogen absorption properties of graphene have been studied by using MD simulations. It is found that under the temperature of 70 K and the pressure of 1 MPa, the hydrogen uptake percentage can be as high as 54%. And the majority of the hydrogen atoms are absorbed during the initial 100 to 200 ps of the simulation. Additionally, the hydrogen storage properties of graphene with different environment temperatures have been studied. We found that with increasing temperature, the hydrogen uptake percentage after reaching the plateau state decreases. Furthermore, the number of layers of the graphene sheet also exerts influence of the hydrogen absorption capability of the sample. We conclude that the more graphene sheets are being used, the less hydrogen atoms are being absorbed by the sample. Our work provides insight into optimizing the environmental temperature and thickness of the graphene sheet when designing novel energy storage devices, especially hydrogen storage devices.

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