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Stability and Electronic property of Vacancy Defects in Silicon Carbide Nanosheet based on DFTB

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Silicon Carbide (SiC) is the chemical compound of carbon and silicon. Recognized as a perfect semiconductor with superior characteristics, SiC is widely used in high-temperature, high-power, and high-frequency electronic applications. Defects in a semiconductor have become a primary important issue since they can damage and change the unwanted electrical properties. The study of geometric and electronic properties of the defects in SiC nanosheet is crucial to understand the effects on an electronic device. In this research, we present a study of the energy gap and formation energy of the defective SiC nanosheet ($Si_{144}C_{144}$) based on self –consistent charge density functional based tight binding (SCC- DFTB) method including van der Waals dispersion corrections. The geometric and electronic properties of defective SiC nanosheet related to the number of vacancy defects in SiC nanosheet have been studied systematically. The defective SiC nanosheet was made by removing Si atoms and C atoms around the central region of SiC nanosheet. The energy gap of pristine SiC nanosheet exhibited 1.060 eV. The energy gap of defect SiC nanosheets were in range of 0.049 to 0.811 eV when Si atoms were removed more than C atoms and 0.028 to 0.753 eV in case of the same rate of removal Si atoms and C atoms. However, when Si atoms were removed less than C atoms, the energy gap showed the less of 0.005 to 0.482 eV. The stability of the SiC nanosheet was investigated by using the calculated normalized formation energies. By increasing vacancy atoms, the defect stability has produced an identical result which is a decline from 75.321 to 87.453 eV. On the other hand, the defect stability has increased (67.722 to 75.504 eV) when vacancy atoms are added to the SiC nanosheet by removing Si atoms less than C atoms. The highest formation energy (87.453 eV) has been found after one single C atom vacancy defect was withdrawn from SiC nanosheet ($Si_{144}C_{143}$) while the lowest formation energy was 67.722 eV when one Si atom was removed ($Si_{143}C_{144}$). We have found that the ratio between the number of silicon atoms and the number of carbon atoms is of the great importance to the stability and electronic properties of the vacancy defect in SiC nanosheet.

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