Two-dimensional Germanane and Germanane Ribbons: Density Functional Calculation of Structural, Electronic, Optical and Transport Properties and the Role of Defects

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1 MD Simulation

We have carried out *ab initio* molecular dynamics (AIMD) simulations by using canonical ensemble (NVT), which is implemented in the Vienna *ab initio* Simulation Package (VASP)[1]. The 4×4 2D sheet is simulated for 5 picosecond (ps) with a time step of 2 femtosecond (fs). The MD calculations were performed at a temperature of 300K for the initially optimized nanostructures at $T = 0K$. The nonspin polarized generalized gradient approximation (GGA) in the form of Perdew-Burke-Ernzerhof (PBE) is used for the exchange-correlation potential[2]. The projector augmented wave (PAW) method and a plane wave basis set with $400eV$ energy cutoff. The convergence criterion of the total energy is set as $10^{-4}eV$. The temperature control is realized by means of Nosé thermostat[3].

The thermal stability of the three nanostructures, i.e., the pristine germanane sheet and the defective germanane with H monovacancy and the defective germanane with Ge adatom, have been investigated. For the three nanostructures mentioned above, it is found that their total energy fluctuations are very small, maintaining in a almost horizontal line. Thus, the MD simulation confirms that all nanostructure under consideration are thermally stable at room temperature.

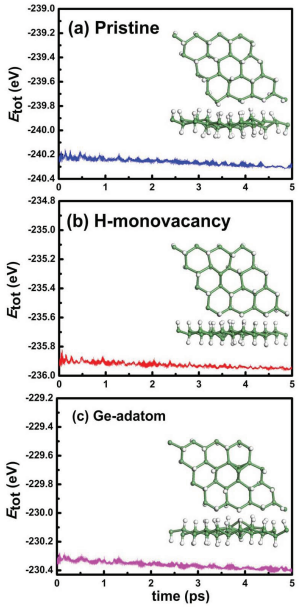

Fig. 1 (Color Online) Total energy fluctuation during AIMD simulations performed at 300K for the (a) pristine germanane sheet and (b) defective germanane with H monovacancy and (c) defective germanane with Ge adatom. The snapshots at the end of simulation are shown in the inset.

References

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