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). 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. The projector augmented wave (PAW) method and a plane wave basis set with 400 eV 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.

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.

References


Corresponding author. E-mail address: zenghui@yangtzeu.edu.cn

![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.