INTI SARI

ENERGI FORMASI DAN DISOSIASI *MULTIVACANCIES* PADA *MONOLAYER* SiC: KOMPUTASI BERBASIS *DENSITY FUNCTIONAL THEORY*

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Studi komputasi *Density Functional Theory* (DFT) digunakan dalam menentukan stabilitas berbagai macam konfigurasi *vacancy* pada silikon karbida (SiC). *Vacancy* dilakukan pada sistem supersel SiC $6 \times 6 \times 1$, dengan 72 atom. *vacancies* dari *mono-* (V_{Si} dan V_C), *divacancy* V1 (V_{SiC}) sampai *vacancy* V7 (V_{Si7C7}) telah dioptimasi. Relaksasi sistem teroptimasi menghasilkan perubahan simetri terhadap konfigurasi *unrelaxed* pada konfigurasi V_C dari simetri D_{3h} menjadi C_{2v}. Memperhitungkan efek relaksasi analisa kestabilan telah dilkukan dengan menghitung nilai energi formasi dan disosiasi menggunakan metode DFT (pada keadaan *unrelaxed* dan relaxed) dan *Dangling Bond Counting Model* (DBCM) pada keadaan *unrelaxed* dalam menganalisa kestabilan sistem. Nilai energi formasi terjadi perubahan pada V_{Si6C6} adanya efek relaksasi berturut-turut adalah 16,99 eV, 16,50 eV, dan 11,92 eV untuk DFT *unrelaxed*, DBCM, dan DFT *relaxed*. Energi formasi menjelaskan kestabilan sistem relatif pada sistem *multivacancies,* kestabilan yang lebih pasti diperoleh dengan perhitungan energi disosiasi. Metode DFT pada keadaan *relaxed* menghasilkan kestabilan sistem dengan memperhitungkan efek relaksasi, dengan energi disosiasi 7,34 eV, V_{Si6C6} menjadi konfigurasi yang paling stabil.

Kata kunci *: silicon carbide*, *density functional theory*, *multivacancies*, energi formasi, energi disosiasi

ABSTRACT

FORMATION AND DISSOCIATION ENERGIES OF MULTIVACANCIES IN MONOLAYER SiC: COMPUTATION BASED ON DENSITY FUNCTIONAL THEORY

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Computational studies using Density Functional Theory (DFT) are used to determine stability in various vacancy configurations of silicon carbide (SiC). Vacancies performed on the SiC supercell system $6 \times 6 \times 1$, with 72 atoms. Vacancies from mono- (V_{Si} and V_C), divacancy V1 (V_{SiC}) to vacancy V7 (V_{Si7C7}) optimized. Relaxation of the optimized system results in a change in symmetry of the unrelaxed configuration in the V_C configuration from D_{3h} to C_{2v} symmetry. Taking into account the relaxation effect, stability analysis has been carried out by calculating the energy value of formation and dissociation using the DFT method (in the unrelaxed and relaxed state) and the Dangling Bond Counting Model (DBCM) in the unrelaxed state in analyzing the stability of the system. The energy value of the formation changed in VSi6C6 with a relaxation effect of 16.99 eV, 16.50 eV, and 11.92 eV consecutively for *DFT unrelaxed*, DBCM, and *DFT relaxed*. Formation energy describes the relative stability of the system in *multivacancies,* more certain stability is obtained by calculating dissociation energy. The DFT method in *the relaxed state* produces system stability by considering the relaxation effect, with a dissociation energy of 7.34 eV, V_{Si6C6} being the most stable configuration.

Keywords: silicon carbide, density functional theory, multivacancies, formation energy, dissociation energy