

INTISARI

KAJIAN STRUKTUR DAN SIFAT ELEKTRONIK MATERIAL DUA DIMENSI *THALLIUM PHOSPHIDE* (TlP) DENGAN KISI SQUARE DENSITY FUNCTIONAL THEORY (DFT)

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Penelitian ini dilakukan untuk mengkaji stabilitas material dua dimensi (2D) *thallium phosphide* (TlP) dengan variasi struktur kisi. Kajian ini penting karena konfigurasi geometris pada material dua dimensi berpotensi menghasilkan sifat elektronik yang berbeda. Stabilitas struktur dianalisis melalui pemodelan dan perhitungan energi total sistem menggunakan pendekatan *Density Functional Theory* (DFT), di mana kondisi stabil dicapai pada energi minimum. Optimasi struktur unit sel dilakukan melalui kalkulasi *self-consistent field* (SCF) dan fitting persamaan keadaan *Birch–Murnaghan* (BM-EOS) untuk memperoleh parameter kisi optimum serta energi kohesif. Sifat elektronik dikaji melalui perhitungan *band structure* dan *projected density of states* (PDOS), serta dianalisis pengaruh *strain* uniaxial dan biaxial terhadap kestabilan dan sifat elektronik material. Hasil penelitian menunjukkan bahwa struktur kisi *square* lebih stabil dibandingkan *honeycomb*, dengan energi kohesif masing-masing sebesar $-6,96$ eV dan $-6,87$ eV. Struktur *square* memiliki konstanta kisi $3,73$ Å dan bersifat planar, sedangkan struktur *honeycomb* memiliki konstanta kisi $4,38$ Å dengan buckling sebesar $2,41$ Å. Secara elektronik, struktur *square* menunjukkan sifat metalik akibat kontribusi orbital P-p di sekitar level Fermi. Pemberian *compressive strain* memperkuat karakter metalik, sedangkan *tensile strain* melemahkannya dan mengindikasikan kecenderungan transisi menuju semikonduktor. Batas kestabilan mekanik struktur ditemukan berada di bawah *strain* $+20\%$, di mana pada kondisi tersebut struktur mengalami kerusakan signifikan.

Kata Kunci: *square*, Sifat Elektronik, *Thallium Phosphide* (TlP), DFT

ABSTRACT

STRUCTURAL AND ELECTRONIC PROPERTIES STUDY OF TWO-DIMENSIONAL THALLIUM PHOSPHIDE (TlP) WITH A SQUARE LATTICE USING DENSITY FUNCTIONAL THEORY (DFT)

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This study aims to investigate the stability of two-dimensional (2D) thallium phosphide (TlP) with different lattice structures. This investigation is important because geometric configurations in two-dimensional materials can lead to distinct electronic properties. Structural stability was analyzed through total energy calculations using the Density Functional Theory (DFT) approach, where the stable condition corresponds to the minimum energy state. The unit cell structure was optimized using self-consistent field (SCF) calculations and fitted with the Birch–Murnaghan equation of state (BM-EOS) to obtain the optimum lattice parameters and cohesive energy. The electronic properties were examined through band structure and projected density of states (PDOS) calculations. Furthermore, uniaxial and biaxial strain were applied to analyze their effects on structural stability and electronic properties. The results show that the square lattice structure is more stable than the honeycomb structure, with cohesive energies of -6.96 eV and -6.87 eV, respectively. The square structure has a lattice constant of 3.73 Å and is planar, whereas the honeycomb structure has a lattice constant of 4.38 Å with a buckling of 2.41 Å. Electronically, the square structure exhibits metallic behavior due to the dominant contribution of P-p orbitals near the Fermi level. The application of compressive strain enhances the metallic character, while tensile strain weakens it and indicates a tendency toward a semiconductor transition. The mechanical stability limit is found to be below +20% strain, beyond which significant structural degradation occurs.

Keywords: Square, Electronic, Thallium Phosphide (TlP), DFT