INTISARI

SPIN SPLITTING PADA SISTEM 1H-WSe_2 *MONOLAYER* DENGAN *POINT DEFECT* : KAJIAN KOMPUTASIONAL BERBASIS *DENSITY FUNCTIONAL THEORY*

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Material *transition metal dichalcogenides* (TMDCs) monolayer memiliki karakteristik *broken inversion symmetry*, efek *spin–orbit interaction* (SOI) yang kuat, serta *valley degree of freedom*, sehingga berpotensi sebagai kandidat material untuk perangkat elektronik generasi lanjut. Penelitian ini mengkaji secara komputasional berbasis *density functional theory* (DFT) sifat elektronik dan spin pada monolayer 1H-WSe_2 dengan sistem *point defect*. Metode *band unfolding* diterapkan untuk mengidentifikasi *defect states* yang terbentuk di sekitar level Fermi. Analisis struktur geometri menunjukkan bahwa sistem dengan *vacancy* Se (V_{Se}) dan *vacancy* W (V_W) masing-masing memiliki simetri *point group* C_{3v} dan C_1, dengan energi formasi yang mengindikasikan V_{Se} lebih stabil dibandingkan V_W. Kemudian, akibat densitas muatan pada V_{Se}, terdapat dua *defect states* di atas level fermi pada sistem V_{Se}, apabila SOI diterapkan maka *defect states* tersebut akan mengalami *splitting*. Kontribusi dominan dari *defect states* sistem V_{Se} terdapat pada orbital NN W-$d_{3z^2-r^2} + d_{xz} + d_{yz}$ dan NN W-$d_{x^2-y^2} + d_{xy}$. Dengan adanya SOI, pada sistem V_{Se} pemisahan level energi pada *splitting* Δ_1 menunjukkan nilai maksimum sebesar 0,13 eV dan *splitting* Δ_2 sebesar 0,086 eV. Perhitungan *spin-resolved band* dan analisis Hamiltonian **k.p** menunjukkan sistem V_{Se} memiliki polarisasi spin kuat pada bidang *out-of-plane* sehingga fenomena *spin-valley locking* tetap terjaga.

Kata kunci : SOI, *point defect*, metode *unfolding*, spintronik, valleytronik, DFT

ABSTRACT

SPIN SPLITTING IN THE 1H-WSe_2 MONOLAYER WITH POINT DEFECT SYSTEM : A COMPUTATIONAL STUDY BASED ON DENSITY FUNCTIONAL THEORY

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Monolayer transition metal dichalcogenides (TMDCs) exhibit broken inversion symmetry, strong spin–orbit interaction (SOI), and a distinct valley degree of freedom, making them promising candidates for next-generation electronic devices. This study presents a computational investigation based on density functional theory (DFT) of the electronic and spin properties of monolayer 1H-WSe_2 with point defects. The band unfolding method is employed to identify defect states formed near the Fermi level. Geometric structure analysis reveals that systems with Se vacancy (V_{Se}) and W vacancy (V_W) possess C_{3v} and C_1 point-group symmetries, respectively, with formation energy calculations indicating that V_{Se} is more stable than V_W. Owing to charge density redistribution in the V_{Se} system, two defect states emerge above the Fermi level. When SOI is included, these states undergo energy splitting with the dominant contributions to the defect states in the VSe system originate from the d orbitals of nearest-neighbor W atoms, specifically the NN W-$d_{3z^2-r^2} + d_{xz} + d_{yz}$ and NN W-$d_{x^2-y^2} + d_{xy}$ orbitals. With the inclusion of SOI, the V_{Se} system shows maximum energy separations of 0.13 eV for splitting Δ_1 and 0.086 eV for splitting Δ_2. Furthermore, spin-resolved band structure calculations and **k.p** Hamiltonian analysis reveal a strong out-of-plane spin polarization in the V_{Se} system, indicating that the spin–valley locking phenomenon remains robust.

Kata kunci : SOI, *point defect*, metode *unfolding*, *spintronics*, *valleytronics*, DFT