INTISARI

KAJIAN KOMPUTASIONAL *VALLEY SPLITTING* PADA SISTEM *HETEROINTERFACE* WSe_2/CoO BERBASIS *DENSITY FUNCTIONAL THEORY*

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Kajian komputasional *valley splitting* pada sistem *heterointerface* WSe_2/CoO dilaksanakan menggunakan metode *density functional theory* (DFT) dengan fungsional *exchange-correlation* Perdew-Burke-Ernzerhof (PBE). Penelitian dimulai dengan mengoptimasi fungsi gelombang Kohn-Sham dengan kriteria konvergensi $2,7 \times 10^{-8}$ eV, dilanjutkan dengan optimasi geometri WSe_2 dan CoO heksagonal dengan kriteria gaya 5×10^{-3} eV/Å. Sistem *heterointerface* yang dikonstruksi terdiri dari 1 lapis monolayer WSe_2 dan 3 lapis CoO heksagonal. Geometri struktur *heterointerface* dioptimasi dengan kriteria gaya yang sama sehingga kestabilan kisi tercapai dengan energi ikat kisi senilai -18,353 eV. Untuk meninjau *valley splitting* pada *heterointerface*, kalkulasi struktur elektronik melibatkan 2 titik simetri tinggi dalam zona Brillouin pertama yaitu K dan K'. Sifat magnetik CoO berpengaruh terhadap keadaan elektronik WSe_2 sehingga memicu pemecahan simetri *time-reversal* yang menyebabkan pemecahan Zeeman pada titik-titik tersebut. Interaksi spin-orbit yang kuat dalam WSe_2 juga berkontribusi pada pemecahan ini. Analisis *spin texture* menunjukkan terjadinya pemecahan *valley* antara titik Q dan Q' senilai 137 meV. Penelitian ini menunjukkan bahwa *valley* dalam monolayer WSe_2 dapat dikendalikan dengan substrat magnetik sehingga cocok untuk aplikasi *valleytronic*.

Kata Kunci : *Density Functional Theory*, *heterointerface*, *valley splitting*.

ABSTRACT

DENSITY FUNCTIONAL THEORY-BASED FIRST-PRINCIPLES STUDY OF VALLEY SPLITTING IN WSe_2/CoO HETEROINTERFACE SYSTEM

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A first-principles study to investigate valley splitting in WSe_2/CoO heterointerface system was conducted using Density Functional Theory (DFT) method. In this work, the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was employed. The calculation began with optimizing the Kohn-Sham wavefunction up to a convergence criteria of 2.7×10^{-8} eV, followed by structural relaxation of WSe_2 and hexagonal CoO using a force convergence criterion of 5×10^{-3} eV/Å. The heterointerface system, consisting of a single WSe_2 layer and 3 hexagonal CoO layers, were also structurally optimized. The system exhibited structural stability with a lattice binding energy of -18.353 eV. To investigate the valley splitting within the heterointerface, high symmetry points within the first Brillouin zone (K and K') were considered during the electronic structure calculation. The magnetic nature of CoO affected the electronic states of WSe_2, breaking the time-reversal symmetry, then inducing Zeeman splittings on the valleys' k-points. Such splittings were also contributed by the strong spin-orbit coupling within WSe_2. Spin texture analysis revealed a 137 meV of splitting was obtained between the Q and Q' valleys. This work suggests that valleys in WSe_2 monolayer can be manipulated using magnetic substrate, making this system a promising candidate for valleytronic applications.

Keywords : Density Functional Theory, heterointerface, valley splitting.