INTISARI

KAJIAN *SPIN-VALLEYTRONIC* PADA MATERIAL *MONOLAYER* TUNGSTEN DIKALKOGENIDA WX_2 (X = S, Se) BERBASIS *DENSITY FUNCTIONAL THEORY*

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Telah dilakukan perhitungan komputasional berbasis *Density Functional Theory* (DFT) pada material *monolayer* WX_2 (X = S, Se) untuk mengetahui karakteristik elektronik dan *valleytronic* material. Perhitungan dimulai dengan melakukan optimasi struktur *monolayer*. Karakteristik elektronik dan valleytronic dapat diketahui dengan menghitung struktur energi, struktur spin, dan *berry curvature* pada material. Hasil kalkulasi struktur energi menunjukkan bahwa material WX_2 miliki *direct band gap* serta terjadi *splitting* energi di K, K' dan Q, Q' *point*. Hasil kalkulasi spin *texture* juga menunjukkan bahwa material *monolayer* WX_2 hanya memiliki polarisasi spin yang mengarah ke komponen z, selain itu juga menunjukkan bahwa material memiliki pasangan valley conduction band minimum (CBM) dan vallence band maximum (VBM) di K, K', dan Q, Q' *point*. Hasil kalkulasi *berry curvature* mengkonfirmasi adanya pasanyan valley VBM pada material di K dan K' *point*. Dari hasil perhitungan komputasi yang telah dilakukan menunjukkan bahwa WS_2 memiliki potensi untuk dijadikan material *spin-valleytronic.*

Kata kunci : *Density Functional Theory*, *monolayer* WX_2 (X = S, Se), struktur energi, *berry curvature,* dan *spin-valleytronic.*

ABSTRACT

SPIN-VALLEYTRONIC SSTUDY ON TUNGSTEN DICHALCOGENIDES WX_2 (X = S, Se) MONOLAYER MATERIAL USING DENSITY FUNCTIONAL THEORY

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Density Functional Theory (DFT)-based computational calculations have been performed on the monolayer material WX_2 (X = S, Se) to determine the electronic and valleytronic characteristics of the material. The calculation starts with optimizing the monolayer structure. Electronic and valleytronic characteristics can be known by calculating the energy structure, spin structure, and berry curvature of the material. The energy structure calculation shows that WX_2 material has a direct band gap and energy splitting occurs at K, K' and Q, Q' points. The spin texture calculation also shows that the WX_2 monolayer material only has spin polarization that leads to the z component, and also shows that the material has valley conduction band minimum (CBM) and vallence band maximum (VBM) pairs at K, K', and Q, Q' points. The results of berry curvature calculations confirm the presence of VBM valley pair in the material at K and K' points. From the results of the computational calculations that have been carried out, it indicates that WS2 has the potential to be used as a spin-valleytronic material.

Keywords : Density Functional Theory, monolayer WX_2 (X = S, Se), energy structure, berry curvature, and spin-valleytronic.