INTISARI

Efek *Strain* Terhadap *Spin Splitting* dan *Spin Textures* Timah Selenium (SnSe) *Monolayer*: Kajian Komputasional Berbasis *Density Functional Theory*

Oleh

Muhammad Anshory
18/433751/PPA/05566

Telah dilakukan kajian komputasi berbasis *density functional theory* (DFT) untuk mengamati struktur elektronik material Timah Selenium (SnSe) *monolayer* pada zona Brillouin pertama akibat pemberian efek *strain*. Penelitian ini menunjukkan adanya fenomena *spin-splitting* di sekitar titik Y dan telah dianalisis menggunakan teori gangguan $\vec{k} \cdot \vec{p}$ dan grup simetri sehingga diperoleh parameter kekuatan interaksi spin-orbit (SOI) untuk sistem SnSe *monolayer*. Berdasarkan hasil perhitungan *spin textures* di sekitar titik Y pada pita konduksi dan pita valensi diperoleh arah orientasi polarisasi spin yang seragam ke arah *out-of-plane*. Selain itu, efek *strain* dapat menyebabkan perubahan nilai distorsi *ferroelectric* pada arah *in-plane* yang merubah besarnya polarisasi listrik internal, sehingga menghasilkan perubahan nilai parameter SOI. Pemberian *uniaxial strain* searah sumbu-x terbukti efektif dalam meningkatkan parameter SOI yaitu mencapai 1.48 eVÅ pada pita konduksi akibat *tensile* 8%. Hasil penelitian ini menegaskan bahwa kontrol parameter SOI dapat dilakukan dengan *strain* tanpa mengubah arah polarisasi spin yang *out-of-plane* menjadikan sistem SnSe *monolayer* sebagai kandidat material *persistent spin helix* (PSH) yang menjanjikan untuk piranti spintronik.

Kata-kata kunci : DFT, PSH, SnSe, *spin-splitting*, *spin textures*, *strain*.

ABSTRACT

Strain Effect on Spin Splitting and Spin Textures of Monolayer Tin Selenide (SnSe): A Computational Study based on Density Functional Theory

By

Muhammad Anshory
18/433751/PPA/05566

A computational research based on density functional theory (DFT) has been carried out to observe the electronic structure of the Tin Selenide (SnSe) monolayer material in the first Brillouin zone under strain effect. This research shows the emerged spin-splitting phenomenon around the Y point, which has been analyzed using the $\vec{k} \cdot \vec{p}$ perturbation theory and symmetry group to obtain the spin-orbit interaction (SOI) parameter for the SnSe monolayer system. Based on the calculation of spin textures on the conduction and valence band around Y point, a uniform spin polarization orientation has been accomplished in the out-of-plane direction. In addition, the strain effect shifts the value of in-plane ferroelectric distortion, which changes the magnitude of internal electric polarization; thus, it affects the magnitude of the SOI parameter. Furthermore, applying uniaxial strain in the x-axis direction is proved effective in increasing the SOI parameter, which reached 1.48 eVÅ in the conduction band due to 8% tensile strength. In conclusion, the results of this research confirm that control of the SOI parameter can be carried out by giving strain without changing the direction of out-of-plane spin polarization; therefore it leads the SnSe monolayer system to be a promising candidate of a persistent spin helix (PSH) material for spintronic devices.

Keywords : DFT, PSH, SnSe, spin-splitting, spin textures, strain.