INTISARI

Kajian Struktur Elektronik pada Monolayer GaTeCl Feroelektrik dengan Pendekatan Komputasional Berbasis *Density Functional Theory* (DFT)

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Perhitungan terhadap struktur elektronik sistem monolayer GaTeCl telah dilakukan di bawah pengaruh *strain* dengan menggunakan pendekatan *Density Functional Theory* (DFT). Pemberian *strain* dibedakan atas *compressive strain* dan *tensile strain*. Hasil perhitungan mengkonfirmasi bahwa pemberian *strain* baik *compressive strain* maupun *tensile strain* memperkecil ukuran celah pita energi dan menurunkan ukuran kopling spin orbit material. Di sisi lain, penambahan *tensile strain* meningkatkan distorsi feroelektrik dalam arah y. Pemberian *tensile strain* yang disertai kopling spin orbit juga mengubah karakter celah pita energi dari *indirect* menjadi *direct.* Analisis terhadap tekstur spin sistem monolayer GaTeCl di dalam ruang kisi balik dengan menggunakan teori gangguan $k \cdot p$ serta konsep simetri mengkonfirmasi keberadaan pemisahan spin dengan tipe *Persistent Spin Texture* (PST). Data distribusi komponen spin dan orientasinya dari perhitungan ini menginformasikan bahwa sistem monolayer GaTeCl hanya mampu menghasilkan polarisasi searah (*unidirectional*) yang reversibel dalam arah z. Besar dan tipe polarisasi spin yang dihasilkan membuktikan bahwa material monolayer GaTeCl terbukti potensial untuk diaplikasikan pada perangkat spintronik.

Kata kunci : Struktur elektronik, polarisasi feroelektrik, tekstur spin, spintronik

ABSTRACT

Electronic Structure Investigation of GaTeCl Monolayer based on Density Functional Theory (DFT)

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A series of calculations of GaTeCl monolayer electronic structure has been carried out under the influence of strain with using Density Functional Theory (DFT) approach. The strain effect is separated into compressive strain and tensile strain. As the result yielded, we confirm that compressive and tensile strain addition reduce the band gap and the magnitude of spin orbit strength. However, the addition of tensile strain also increases ferroelectric distortion in y direction. The insertion tensile strain in conjunction with spin orbit coupling changes the bandgap from indirect to direct character as well. In contrast to that, by applying $k \cdot p$ perturbation theory and symmetry group, spin texture analysis confirms the existence of Persistent Spin Texture (PST) type of splitting in Γ point VBM. The spin components distribution data and their orientation from these calculations inform that the system solely has uni-directional polarization which is reversible in z direction. The magnitude and spin polarization type produced prove that monolayer GaTeCl is applicable for the realization of spintronics devices.

Keywords : Electronic structure, ferroelectric polarization, spin texture, spintronics