

INTISARI

**STRUKTUR ELEKTRONIK MoX₂ (X=S, Se, Te) *MONOLAYER*:
KAJIAN TEORITIK KOMPUTASIONAL BERBASIS *DENSITY*
*FUNCTIONAL THEORY***

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Telah diamati efek *spin-orbit coupling* (SOC) pada struktur elektronik material MoX₂ (X=S, Se, Te) *monolayer* dengan pendekatan *Density Functional Theory* (DFT). Hasil perhitungan menunjukkan bahwa ditemukan *spin-splitting* sepanjang garis K- Γ yang disebabkan karena pecahnya *inversion symmetry* pada struktur kristal MoX₂ *monolayer*. Sedangkan disepanjang garis Γ -M tidak terdapat *spin-splitting* yang disebabkan oleh *time reversability* dan *mirror symmetry*. Pengaruh medan listrik luar diberikan pada struktur elektronik MoX₂ *monolayer* untuk mengetahui evolusi struktur elektronik. Hasil yang diperoleh menunjukkan adanya *spin-splitting* pada arah Γ -M sehingga menghasilkan efek Rashba disekitar titik Γ . Selain itu, pengaruh medan listrik luar juga mengakibatkan adanya transisi dari *direct* ke *indirect band gaps* dan menghasilkan transisi dari semikonduktor ke logam ketika medan listrik yang diberikan semakin besar. Munculnya *spin-splitting* pada struktur elektronik material MoX₂ menunjukkan bahwa material MoX₂ sangat potensial untuk divais spintronik.

Kata kunci: MoX₂ *monolayer*, *spin-splitting*, DFT, SOC

ABSTRACT

ELECTRONIC STRUCTURE MONOLAYER MoX₂ (X=S, Se, Te): A THEORETIC-COMPUTATIONAL STUDY BASED ON DENSITY FUNCTIONAL THEORY

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We have observed spin-orbit coupling (SOC) effects on the electronic structure of MoX₂ (X = S, Se, Te) monolayer material with Density Functional Theory (DFT) approach. The calculations show that spin-splitting is found along the K-garis line caused by the broken of inversion symmetry in the crystal structure of MoX₂ monolayer. While along the line Γ -M, there is no spin-splitting due to the time reversability and mirrors symmetry. External electric field effect is applied on the electronic structure of MoX₂ monolayer to investigate evolution of electronic structure. The results show the spin-splitting in the Γ -M direction, and thus inducing rashba effects around the point Γ . In addition, external electric field effect also resulted in the transition from direct to indirect band gaps, which induced transition from semiconductor to metal when the electric field provided is getting bigger. The appearance of spin-splitting on the electronic structure of MoX₂ material shows that the MoX₂ material is highly potential for spintronic devices.

Keyword: MoX₂ monolayer, spin-splitting, DFT, SOC