INTISARI

EFEK HALL ANOMALI PADA SISTEM FeX_2 (X= Cl, Br, I) DUA DIMENSI: KAJIAN KOMPUTASIONAL MENGGUNAKAN *DENSITY FUNCTIONAL THEORY*

Oleh:

ARIFIA PRATIWI NUGRAHENI

20/459194/PA/19855

Telah dilakukan kajian komputasional berbasis *Density Functional Theory* (DFT) pada sistem 1T-FeX_2 (X= Cl, Br, I) untuk menyelidiki efek *Hall* anomali. Perhitungan dilakukan melalui serangkaian tahapan yang meliputi optimasi struktur geometri, kalkulasi struktur elektronik tanpa dan dengan *spin-orbit coupling*, *Berry curvature*, dan konduktivitas Hall anomali (AHC). Kalkulasi struktur elektronik dengan pendekatan *colinear* DFT menghasilkan struktur pita energi dengan titik *Weyl* dan pita yang sangat berdekatan di sekitar *Fermi level*. Kalkulasi struktur elektronik dengan pendekatan *non-colinear* DFT menghasilkan bukaan celah baru dan pelebaran celah yang bervariasi terhadap orientasi spin (θ). Lokasi celah tersebut bersesuaian dengan puncak-puncak *Berry curvature* dan membentuk puncak-puncak AHC. Nilai AHC di *Fermi level* masing-masing material sebesar $0{,}06\ e^2/h$, $-0{,}27\ e^2/h$, dan $-0{,}55\ e^2/h$. Perubahan anion Cl, Br, I menghasilkan nilai AHC yang lebih besar hingga di atas 9 kali lipat. Dua puncak pertama AHC di dekat *Fermi level* bernilai besar dan anisotropi. Perubahan sudut θ menyebabkan puncak AHC berbalik saat melampaui $90°$. Dua puncak AHC menghasilkan kemiringan kurva di sekitar *Fermi level* sehingga berpotensi untuk diaplikasikan dalam sistem spin-termoelektrik berbasis efek Nernst.

Kata kunci: DFT, *monolayer* 1T-FeX_2, orientasi spin, struktur elektronik, *Berry curvature*, konduktivitas *Hall* anomali.

ABSTRACT

ANOMALOUS HALL EFFECT ON TWO DIMENSIONAL $Fe X_2$ (X= Cl, Br, I) SYSTEMS: A COMPUTATIONAL STUDY USING DENSITY FUNCTIONAL THEORY

By:

ARIFIA PRATIWI NUGRAHENI

20/459194/PA/19855

A Density Functional Theory (DFT) study has been done to investigate the Anomalous Hall Effect on 1T-FeX_2 (X= Cl, Br, I) systems. The calculation was carried out on a series of steps, including geometric structure optimization, calculation of electronic structure with and without spin-orbit coupling, Berry curvature, and anomalous Hall conductivity (AHC). Electronic structure calculation with colinear DFT resulted in band structure with Weyl point and adjacent bands around the Fermi level. Electronic structure calculation with colinear DFT brought on the new open gap and the gap widening which varies with spin orientation (θ). The gap location corresponds to Berry curvature peaks and gave rise to the AHC peaks. AHC values in the Fermi level were $0{,}06\ e^2/h$, $-0{,}27\ e^2/h$, and $-0{,}55\ e^2/h$ respectively. The anion Cl, Br, I substitution generated over 9 times larger AHC. The two first AHC peaks near Fermi level have large values and are anisotropic. The θ angle change led to inversing AHC peaks when passing above 90°. Two peaks led to a slope of the AHC curve around Fermi level, so that potential for application in the Nernst effect-based spin-thermoelectric system.

Keywords: DFT, 1T-FeX_2 monolayers, spin orientation, electronic structure, Berry curvature, anomalous Hall conductivity.