Chanul Kim[1]

Seyoung Park[2,3], Youngwoo Son[1] Co-Authors (Arial Narrow 16)

1. Korea Institute for Advanced Study, 85 Hoegiro, Dongdaemun-gu, Seoul, South Korea
2. Institute for Basic Science, 1 Gwankak-ro, Gwanak-gu, Seoul, South Korea
3. Seoul National University, 1 Gwankak-ro, Gwanak-gu, Seoul, South Korea

chanulkim@kias.re.kr

First-principles study on the intrinsic origin of the large anomalous Hall effect in perovskite $La_{1-x}Sr_xCoO_3$

We investigate the electronic and transport properties of perovskite $La_{1-x}Sr_xCoO_3$, in which the large anomalous Hall effect (AHE) is reported with strong doping dependences. Using first-principles density functional plus U (DFT+U) method, we find the significant change in the band character of Co-d derived bands with respect to the Fermi level shift. Without spin-orbit coupling (SOC), we identify the doubly degenerate nodal lines near the Fermi energy, protected by inversion and three-fold rotation symmetry. We find that the inclusion of the spin-orbit coupling lifts the degeneracy with peak in the Berry curvature, which induces large variation of the calculated anomalous Hall effect depending on the position of Fermi energy. Our finding suggests the intrinsic origin of the large anomalous Hall effects in $La_{1-x}Sr_xCoO_3$ and further provides an effective way to identify the materials with large anomalous Hall effect from the space group symmetry.

References

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