Ab-initio Hall Factor Formulation and Its Application in Functional Group Identification of Semiconducting MXenes

Satadeep Bhattacharjee,[1*] Anup Kumar Mandia,[2] Namitha Anna Koshi,[1] Bhaskaran Muralidharan,[2] and Seung-Cheol Lee,[1,3]

[1] *Indo Korea Science and Technology Center, Bangalore (IKST)*
[2] *Indian Institute of Technology, Bombay (IIT-Bombay)*
[3] *Korea institute of Science and Technology (KIST)*

This presentation will cover an integrated methodological development and its application to investigate magneto-transport phenomena in semiconducting MXenes. Initially, I will introduce an ab-initio calculation framework for the Hall factor, developed by incorporating Rode's iterative technique within density functional theory (DFT). Utilizing this approach, we find notable temperature and carrier concentration-dependent deviations of the Hall factor from unity in Ti_2CO_2, highlighting the critical importance of such corrections in accurately extracting drift mobility and carrier densities. Subsequently, the methodology is generalized to Sc-based MXenes (Sc_2CF_2, Sc_2CO_2, $Sc_2C(OH)_2$), revealing distinctive Hall factor signatures associated with different surface functional groups. This extension offers a robust and physically insightful approach to experimentally distinguish surface functional groups in MXenes, effectively integrating methodological innovation with precise materials characterization.

References

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