First-principles methodology for Magneto-transport properties of real materials

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In this report, we detail a methodology that merges first-principles calculations with semiclassical Boltzmann transport theory, implemented through the open-source software WannierTools, to study magnetoresistance and Hall effects in a range of materials such as non-magnetic metals, semimetals, semiconductors, and magnetic metals. We explore the scaling behavior of Hall effects in response to changes in temperature and magnetic fields and show how this approach successfully interprets anomalous rho-T curves influenced by magnetic fields. This research enriches our understanding of magnetotransport properties and highlights the importance of theoretical frameworks in decoding experimental results. Our findings not only enhance our knowledge of magnetic materials but also pave new pathways for their scientific classification and practical application.

References：

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