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Efficient Ab-initio Calculation of the Anomalous Hall Conductivity of Fe by Wannier Interpolation XINJIE WANG, DAVID VANDERBILT, Rutgers University, JONATHAN YATES, IVO SOUZA, LBNL and University of California, Berkeley — Recently, a first-principles calculation of the anomalous Hall conductivity (AHC) of Fe as a Brillouin-zone integral of the Berry curvature was carried out and found to be in reasonable agreement with experimental results.[1] However, these authors observed extraordinarily strong and rapid variations of the Berry curvature with wavevector k in the vicinity of avoided crossings and near-degeneracies in reciprocal space. A conventional first-principles calculation thus requires an extremely dense k-point mesh and is quite time-consuming. Here, we present an efficient first-principles approach for computing the AHC based on Wannier interpolation. First, a conventional electronic-structure calculation is performed for Fe, with spin-orbit included, on a relatively coarse k-point mesh. Second, maximally-localized Wannier functions are constructed by a post-processing step,[2] thus transforming the full ab-initio problem into an effective tight- binding form. Finally, the needed quantities such as Berry potentials and curvatures are interpolated onto a fine k-point mesh and used to compute the AHC. Our approach gives good agreement with conventional, less efficient first-priciples calculations.

[1]Y. Yao *et al.*, Phys. Rev. Lett. **92**, 037204 (2004).
[2]I. Souza,N. Marzari, and D. Vanderbilt, Phys. Rev. B **65**, 035109 (2001).

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