Dependence of anomalous Hall effect on spin-orbit coupling strength in bcc Fe

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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. Since the AHC vanishes in the limit of zero spin-orbit (SO) coupling, it is interesting to understand the behavior of the AHC as the SO coupling strength is artificially varied. We investigate this question working in the context of a Wannier interpolation approach to the calculation of the bandstructure and the AHC. The SO coupling strength is varied by tuning the projectors and their coefficients in the fully relativistic norm-conserving pseudopotential, which takes the form of a spatially-dependent 2×2 matrix acting on spinor wavefunctions. In this way we separately control the strength λ_z of the spin-diagonal components and that of the spin-off-diagonal components λ_{xy} of the pseudopotential. The calculated AHC is found to be an odd function of λ_z and an even function of λ_{xy}, with both linear and quadratic components playing a significant role in both cases. The existence of a contribution scaling as $|\lambda_{xy}|$ is surprising from the viewpoint of conventional perturbation theory.

[1] Y. Yao *et al.*, Phys. Rev. Lett. **92** 037204 (2004).