**Revisiting Anomalous Hall Conductivity in BCC Iron via First-Principles Tight-Binding Calculations using Pseudo Atomic Orbitals**

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The frequency-dependent Hall conductivity in ferromagnetic bcc Fe serves as a standard example for benchmarking the first-principles calculations based on a variety of different approaches. So far the first-principles calculations obtained via the generalized gradient approximation have been found to well describe the available experimental data [1,2]. In the poster presentation, we will show that better agreement with the magnetic circular dichroism experiments can be reached once the effect of the bandwidth renormalization [3] is taken into account. We will also present how to calculate the frequency-dependent optical conductivity based on the first-principles tight-binding Hamiltonian that is straightforwardly obtained after finishing a self-consistent calculation using the bases of pseudo atomic orbitals implemented in the OpenMX code [4]. In particular, a general formula without assuming the orthonormal relation between orbitals for calculating the momentum matrix elements needed for obtaining the conductivity based on the Kubo-Greenwood formula will be given. The position matrix elements will be demonstrated to be important for delivering the exact momentum matrix elements. We note that the only needed information in the derived formula is the position matrix element and the ingredients that have already contained in the tight-binding representation, evidencing the usefulness of the derived formula.

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2. Jonathan R. Yates *et al*., Phys. Rev. B **75**, 195121 (2007).
3. Tobias Schickling *et al*., Phys. Rev. B **93**, 205151 (2016).
4. Chi-Cheng Lee *et al*., Phys. Rev. B **98**, 115115 (2018).