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Ab-initio **calculation of electron-phonon coupling for spin relaxation in metals.** MIGUEL PRUNEDA, UC Berkeley & ICMAB, IVO SOUZA, UC Berkeley — Spin-electronic devices have motivated an important effort in understanding the mechanisms for spin-relaxation, because the operation of such devices requires long spin-diffusion lenghts. Two main factors contribute to spin relaxation: (i) spin-orbit interaction, which mixes the spin-up and spin-down components of the electronic wavefunction, and (ii) electron scattering from defects or phonons. In metals, the phonon-mediated Elliot-Yafet mechanism is believed to be dominant. Realistic calculations are computationally demanding,[1] requiring an accurate description of the electronic states near the Fermi surface and their coupling to the lattice (phonons). Here we use a Density Functional Perturbation Theory implementation to calculate from first-principles the electron-phonon interaction in systems with spin-orbit coupling. Combined with recently-developed Wannier-interpolation methods for sampling efficiently the Brillouin zone, this will allow for a fully *ab-initio* calculation of the spin relaxation in metals.

[1]J. Fabian and S. Das Sarma, *Phys. Rev. Lett.* **83**, 1211 (1999).

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