Frontiers of First-Principles Electron-Phonon Interactions: Spinful, Data-Driven, and Parsimonious

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Electron-phonon (e-ph) interactions have become a pillar of first-principles electronic structure calculations. In this talk, I will introduce relevant theory and computational workflows, and then I will highlight two emerging frontiers of e-ph calculations: (i) Precise calculations of spin-phonon interactions and spin relaxation; (ii) data-driven methods to compress e-ph interactions, significantly speed-up their computation, and achieve parsimonious / Pareto-optimal models. To conclude I will discuss advances in our open source code, PERTURBO, which makes these new computational methods available to the community.