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**Correlation-enhanced electron-phonon coupling**[1]

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Electron-phonon coupling (EPC) plays an important role in many material properties such as resistivity and conventional superconductivity. Accurate theoretical calculations of EPC in solids is essential for computational design, discovery and optimization of many functional materials. The widely used density functional theory (DFT) in the local density approximation (LDA) and generalized gradient approximation (GGA) can reasonably compute the EPC in weakly correlated materials but suffers from important shortcomings in strongly correlated materials. The self-energy of the quasiparticles in correlated materials modifies the LDA/GGA electronic structures hence the phonon frequencies and EPC. In this talk, I will discuss two types of underestimation of the EPC by LDA/GGA and propose a simple yet efficient methodology to evaluate the realistic EPC by using advanced electronic structure method beyond LDA/GGA. The extraordinarily high superconducting temperatures that are observed in two distinct classes of compounds–the bismuthates and the transition-metal chloronitrides can be readily accounted for by the correlation-enhanced EPC. Further impact of electronic correlation on the coupling of phonons and electronic degrees of freedom will also be discussed.

Reference: Z. P. Yin, A. Kutepov, and G. Kotliar, Phys. Rev. X 3, 021011 (2013).

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