

Electron-Phonon Interactions in Correlated Materials from Dynamical Mean-Field Theory

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First-principles calculations of electron-phonon coupling and phonon-mediated transport effects have become a centerpiece of modern computational materials physics, with many successful demonstrations of electrical transport predictions in conventional materials systems. In strongly correlated electron materials, however, electron-electron interactions can lead to a dramatic enhancement or suppression of electron-phonon coupling [1,2], altering critical properties including electrical conductivity and superconducting critical temperature. Dynamical mean-field theory can describe electron correlation effects in materials where DFT and perturbative approaches fail, but so far, has not been used in a systematic way to predict electron-phonon coupling. In this talk, I will outline multiple DFT+DMFT approaches to account for the effect of correlations on first-principles electron-phonon matrix elements, including by frozen phonon and linear response methods, and provide demonstrations of these methods for material calculations.

[1] D. Abramovitch, J. Coulter, S. Beck, A. Millis. Phys. Rev. B 112, 075113 (2026).

[2] J. Coulter, A. Millis. Phys. Rev. B 113, 165145 (2025).