Ab initio modeling of superconductivity in materials with the anisotropic Migdal-Eliashberg formalism

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The coupling between electrons and phonons plays a central role in defining technologically important materials properties, from charge and heat transport to superconductivity and light-driven phase transitions. Recent advances in computational methodology based on maximally-localized Wannier functions have enabled efficient calculations of electron–phonon matrix elements on ultra-dense momentum grids. My group has been leading the effort dedicated to the implementation and consolidation of the anisotropic Wannier-based Migdal-Eliashberg formalism for modeling phonon-mediated superconductors in the open-source EPW package. The methodology allows one to perform highly accurate calculations of the anisotropic temperature-dependent superconducting gap and critical temperature. In this talk, I will highlight recently implemented features in EPW and examples of predicted conventional high-temperature superconductors synthesizable under ambient conditions.

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