

Abstract Submitted
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Using atomic orbitals to compute and interpolate the electron-phonon interaction LUIS AGAPITO, MARCO BERNARDI, Department of Applied Physics and Materials Science, California Institute of Technology — The electron-phonon interaction (EPI) controls key dynamical properties in materials, including charge and spin transport, and ultrafast carrier dynamics. Accurately computing these properties involves obtaining the EPI on very fine Brillouin zone (BZ) grids; since direct ab initio computation is prohibitively expensive, schemes to interpolate the EPI are needed. We present a new method that uses atomic-orbitals (AOs) to compute and interpolate the EPI on fine BZ grids, with important advantages over the alternative Wannier function (WF) interpolation. Different from WFs, AOs are readily available from databases. Their use can be automated without the trial-and-error optimization required in WFs, making AOs suitable for high-throughput study of carrier dynamics in materials. We will discuss the formalism and numerical implementation of our approach, comparing computational cost and accuracy with WFs. The impact of the completeness of the AO set (i.e., single zeta, double zeta, etc.) on the accuracy will be analyzed. Applications to complex materials for which WFs are not ideally suited will be discussed, along with processes that are naturally mapped onto AO sets, such as polaron transport in conjugated molecules and correlated oxides.

Luis Agapito
California Institute of Technology

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