Unraveling s-d scattering mechanisms in crystalline transition metals from ab initio calculations

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We propose an ab initio framework combining maximally localized Wannier functions and Allen's method to accurately model inter-orbital hybridization in crystalline transition metals. Using Wannier-projected orbital weights, we decompose transport spectral functions into distinct scattering channels without artificially isolating pure band manifolds. Applied to fcc Pd and bcc Mo, we rigorously validate this decomposition, showing that the parallel addition of orbital channels perfectly reproduces full calculations. We reveal that the absence of a d-band peak at the Fermi level in Mo enhances s-s scattering, while the s-s contribution in Pd quantitatively matches experimental data for Ag. Additionally, accounting for thermal expansion proves essential for high-temperature accuracy. Ultimately, this hybridized approach eliminates standard disentanglement artifacts, providing a universal tool for analyzing electron-phonon scattering in strongly hybridized systems.