Ab initio extracting of separate electronic contributions to transition metals' transport properties

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The *s*-*d* scattering mechanism, first proposed by Mott [1], is the dominant source of electrical resistivity in transition metals, primarily driven by electron–phonon interactions. Accurate modeling of *s*-*d* electronic transitions is essential for understanding processes under ultrafast laser pulses in thin metallic films. Allen's approach to transport properties calculations [2] applies broadly across metals and successfully reproduces the unusual nonlinear temperature dependence of resistivity in several transition metals. It has been suggested [3] that the ρ_{ss} contribution—where both initial and final scattering states are *s*-like—in Pd can be approximated by the resistivity of Ag—the nearest non-transition-metal neighbor of Pd. In this work, we consider several criteria for distinguishing Bloch states of *s*- and *d*-type to more accurately select strongly hybridized states close to the chemical potential. We compute separate electronic contributions to total resistivity of Pd using Allen's method built upon *ab initio* calculations and Wannier interpolation as implemented in our `SKiES` code [2]. The results presented for both electrical resistivity and phonon linewidth in Pd.

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