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Implementation of Electron-Phonon Coupling in the KKR Formalism and its Applications to Simple Metals CARSTEN EBERHARD MAHR, MICHAEL CZERNER, CHRISTIAN FRANZ, CHRISTIAN HEILIGER, Institute of Theoretical Physics, Justus-Liebig-University, Giessen, Germany — Electron-phonon coupling is one of the main incoherent inelastic scattering mechanisms in a wide variety of crystalline material systems at room temperature. Therefore, it is necessary to incorporate those effects in any realistic calculation of thermoelectric properties. We do so by extending our density functional theory (DFT) based Korringa-Kohn-Rostocker (KKR) Green's function formalism code. By approximating the Fröhlich-type interaction with a self-energy $\Sigma_{eph} = -i\frac{\hbar}{2\tau}$ we are able to compute the dressed propagator G by solving Dyson's equation $G = G_{ref} + G_{ref} \cdot (\Delta V + \Sigma_{eph}) \cdot G$, where G_{ref} is the Green's Function of an arbitrary (though typically repulsive) reference system. The corresponding electron-phonon scattering time τ is extracted from electron linewidth calculations. We demonstrate the physical validity of the beforementioned calculational scheme for non-equilibrium properties by comparing evaluated temperature dependent resistivity characteristics of transport systems consisting of copper, aluminum and other simple metals to experiment. Further, technical details of the implementation in the KKR basis set are presented.

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