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Optical Absorption Spectrum of Gold from First Principles[1] JAMAL MUSTAFA, University of California at Berkeley, Lawrence Berkeley National Lab, EMMANOUIL KIOUPAKIS, University of Michigan, STEVEN LOUIE, University of California at Berkeley, Lawrence Berkeley National Lab — Phonon-assisted optical absorption is an important optical process in metals for photons in the visible part of the spectrum. Developments in first-principles computational methods have enabled the calculation of phonon-mediated optical absorption spectra of materials. The use of Maximally Localized Wannier Functions enables the interpolation of the GW quasiparticle band structure, along with the optical and electron-phonon coupling matrix elements, to very fine meshes in the Brillouin zone, which are needed for the calculation of the phonon-assisted absorption coefficient. We present calculations on gold that include the quasiparticle band structure and lifetimes, phonon dispersion, Wannier functions, and the phonon-assisted absorption spectrum. Since indirect absorption is a second-order process, the lifetime of the virtual intermediate state is of central importance. The results are compared to experimentally determined optical constants.

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