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Inclusion of the electron-phonon interaction in the BerkeleyGW computational package[1] DEREK VIGIL-FOWLER, STEPHAN LANY, Natl Renewable Energy Lab — The BerkeleyGW package is a highly optimized and efficient code for calculating, among others, the dielectric response, bandstructures, lifetimes, and optical absorption of materials from nanostructures and two-dimensional sheets to bulk materials. In the past the only interactions included in BerkeleyGW were electron-electron interactions, with other packages being used to include the effect of, say, electron-phonon interactions. One common approach is to use Wannier functions to interpolate all needed quantities to a very fine grids in energy and momentum, which leads to very accurate electron-phonon couplings and lifetimes. However, in materials with complex, even unknown, chemical environments the generation of Wannier functions can be quite time consuming and constitutes another step in an already difficult calculation. The BerkeleyGW package has a wavefunction-based interpolation scheme that is used in solving the Bethe-Salpeter equation and which is much more easily automated than Wannier interpolation. In this talk, we discuss results for the carrier lifetimes due to the electron-phonon interaction using this interpolation scheme. In particular, we discuss the computational efficiency and scalability, and the prospects for applying this method to a wide range of materials to get first principles lifetimes, and related quantities, such as mobilities and diffusion lengths.

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