Abstract Submitted
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Ab Initio Electronic Relaxation Times and Transport in Noble Metals[1] JAMAL I. MUSTAFA, University of California at Berkeley and Lawrence Berkeley National Lab, MARCO BERNARDI, California Institute of Technology, JEFFREY B. NEATON, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Relaxation times employed to study electron transport in metals are typically assumed to be constants and obtained empirically using the Drude model. Here, we employ ab initio calculations to compute the electron-phonon relaxation times of Cu, Ag, and Au, and find that they vary significantly on the Fermi surface, spanning $\sim$15$-$45 fs. We compute room temperature resistivities in excellent agreement with experiment by combining *GW* bandstructures, Wannier-interpolated band velocities, and ab initio relaxation times. Our calculations are compared to other approximations used for the relaxation times. Additionally, an importance sampling scheme is introduced to speed up the convergence of resistivity and transport calculations by sampling directly points on the Fermi surface.

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