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Ab initio Electron Mobility and Polar Phonon Scattering in GaAs[1] JIN-JIAN ZHOU, MARCO BERNARDI, California Institute of Technology — In polar semiconductors and oxides, the long-range nature of the electron-phonon (e-ph) interaction is a bottleneck to compute charge transport from first principles. Here, we develop an efficient ab initio scheme to compute and converge the e-ph relaxation times (RTs) and electron mobility in polar materials. We apply our approach to GaAs, where using the Boltzmann equation with state-dependent RTs, we compute mobilities in excellent agreement with experiment at $250-500$ K. The e-ph RTs and the phonon contributions to intra-valley and inter-valley e-ph scattering are also analyzed. Our work enables efficient ab initio computations of transport and carrier dynamics in polar materials.

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