Fully Ab initio Electron Mobility and Polar Optical Phonon Scattering in GaAs

DRAFT ABSTRACT

Background and motivation	Polar optical phonon (POP) scattering of electron and carrier mobility in polar semiconductors are typically studied via a simplified empirical model.
Solution	Here we present fully *ab initio* calculations of electron mobility and intravalley relaxation times dominated by POP scattering in pure GaAs. We develop an efficient scheme to converge the relaxation times and mobility which yields an excellent agreement with experimental results.
Results	Our calculations indicate the relaxation time approximation with state-dependent relaxation times produces accurate values for the electron mobility from 250K to 450K, contrary to previous works employing an empirical model. Furthermore, we find electronic states within a small energy regime, whose scattering dominated by POP absorption, contribute significantly to transport.
Significance and broader implications	The parameter-free and predictive computational approach demonstrated here enables *ab initio* studies of carrier dynamics and transport in advanced polar materials.
Specific question / knowledge gap (omitted)	

In this first draft, the abstract background begins at a level that is too specific and would not be understood by a wide scientific audience (which is necessary to recruit as many readers as possible). The specific question / knowledge gap the authors are trying to solve is not explicitly stated. The results sentences are wordy and inefficient.

Thanks to Marco Bernardi for use of this abstract.

HWC
The Hixon Writing Center at Caltech

Ab initio Electron Mobility and Polar Phonon Scattering in GaAs

SUBMITTED ABSTRACT

Background and motivation

Specific question / knowledge gap

Solution

Results

Significance and broader implications

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.

The submitted abstract does a good job of following the hourglass structure and it has omitted unnecessary words present in the first draft. It begins with a background statement that is sufficiently broad to capture wide readership. The question/knowledge gap is specific and the solution to that problem is explicitly stated. Only the major results are highlighted and the immediate implications of the results are stated. The abstract might benefit from one additional statement regarding the broader significance of the work.

Thanks to Marco Bernardi for use of this abstract.

HWC
The Hixon Writing Center at Caltech