aMoBT: *ab initio* Model for Calculating Mobility Using Boltzmann Transport (PV-4)

A joint India-U.S. research consortium funded under the *Joint Clean Energy Research & Development Center (JCERDC)*

Scientific Achievement:

We developed a new, first-principles model to directly calculate electronic transport properties (e.g., mobility, conductivity, Seebeck coefficient) of semiconductors.

Significance and Impact:

The fully predictive model enables high-throughput screening of new materials and also provides insight on transport limitations that hinder performance. aMoBT is available for public use on nanoHub and at http://www.seriius.org/modeling.html.

Research Details:

- The Boltzmann transport equation is linearized and solved directly to calculate the mobility, conductivity, and Seebeck coefficient of semiconductors such as GaAs (Fig. 1) and InN (Fig. 2).
- Hybrid density functional theory calculations are used to obtain the accurate electronic band structure and other necessary parameters, using only the crystal structure of the semiconductor material.
- Both elastic and inelastic scattering mechanisms—including polar optical phonon, ionized impurity, piezoelectric, deformation potential, and scattering from dislocation defects—are explicitly treated in the model.
- The research is a collaboration between Washington University in St. Louis and Lawrence Berkeley National Laboratory.

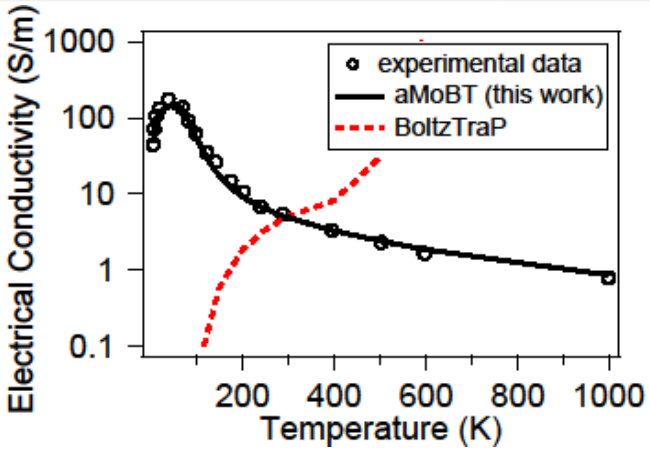

Fig. 1. Electrical conductivity of GaAs

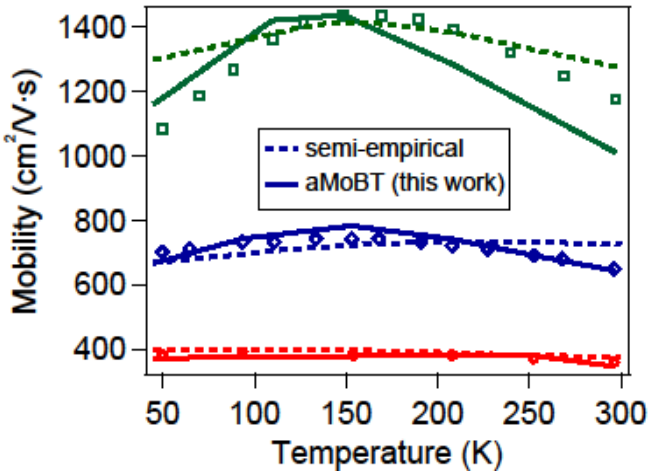

Fig. 2. Mobility of InN: calculated vs. exp.

Publication: "Ab Initio Electronic Transport Model with Explicit Solution to the Linearized Boltzmann Transport Equation," A. Faghaninia, J.W. Ager III, and C.S. Lo, *Physical Review B, Condensed Matter and Materials Physics* **91** 235123 (2015).
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