**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](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.

DOI: [http://dx.doi.org/10.1103/PhysRevB.91.235123](http://dx.doi.org/10.1103/PhysRevB.91.235123)

**Contact:** Cynthia S. Lo (clo@wustl.edu)