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First-principles carrier transport using the Boltzmann Transport Equation in EPW[1] SAMUEL PONCÉ, University of Oxford, ELENA ROXANA MARGINE, Binghamton University, State University of New York, FELICIANO GIUSTINO, University of Oxford — Understanding transport and carrier mobilities in semiconductors is crucial in electronics, optoelectronics, and energy applications. To predict mobilities in theoretical (not yet made) materials would be a remarkable achievement. Fully predictive first-principles calculations of mobilities have only been made possible recently with the advance of ab-initio tools to compute electron-phonon interactions with high accuracy. Here, we present a comprehensive framework to study electron and hole transport in metals and insulators within the full self-consistent linearized Boltzmann transport equation and its approximations. The theory is implemented into the free and open-source code EPW [1,2]. We study four representative semiconductors: Si, GaAs, GaN and bulk MoS_2 and discuss challenges associated with ultra dense sampling and polar electron-phonon interactions.
[1] S. Poncé *et al.*, Comput. Phys. Commun. **209**, 116 (2016)
[2] http://epw.org.uk

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