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First-principles calculations of mobility

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First-principles calculations can be a powerful predictive tool for studying, modeling and understanding the fundamental scattering mechanisms impacting carrier transport in materials. In the past, calculations have provided important qualitative insights, but numerical accuracy has been limited due to computational challenges. In this talk, we will discuss some of the challenges involved in calculating electron-phonon scattering and carrier mobility, and outline approaches to overcome them. Topics will include the limitations of models for electron-phonon interaction, the importance of grid sampling, and the use of Gaussian smearing to replace energy-conserving delta functions. Using prototypical examples of oxides that are of technological importance—$SrTiO_3$ [1], $BaSnO_3$ [2], Ga_2O_3, and WO_3—we will demonstrate computational approaches to overcome these challenges and improve the accuracy. One approach that leads to a distinct improvement in the accuracy is the use of analytic functions for the band dispersion, which allows for an exact solution of the energy-conserving delta function. For select cases, we also discuss direct quantitative comparisons with experimental results. The computational approaches and methodologies discussed in the talk are general and applicable to other materials, and greatly improve the numerical accuracy of the calculated transport properties, such as carrier mobility, conductivity and Seebeck coefficient. This work was performed in collaboration with B. Himmetoglu, Y. Kang, W. Wang, A. Janotti and C. G. Van de Walle, and supported by the LEAST Center, the ONR EXEDE MURI, and NSF. [1] B. Himmetoglu, A. Janotti, H. Peelaers, A. Alkauskas, and C.G. Van de Walle, *Phys. Rev. B* **90**, 241204 (2014). [2] K. Krishnaswamy, B. Himmetoglu, Y. Kang, A. Janotti, C. G. Van de Walle, *eprint arXiv*:1610.06253 (2016).

[1]This is the abstract for an invited talk in Session K8, Talk K8.00001.