May 17, 2021 10:00 AM
QED & Materials seminar
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Title
"Ab initio electron-defect interactions and defect-limited carrier mobility in solid-state materials"

Abstract
Crystallographic defects and impurities govern charge transport at low temperatures, where the electron-defect (e-d) interactions limit the carrier mobility and manifest themselves in a wide range of phenomena of broad relevance in condensed matter physics. Theoretical treatments of e-d interactions have so far relied on heuristic approaches and analytic models. However, the band structure, electronic wave functions, and defect perturbation potential are far more complex in real materials than in these simplified models.

First-principles calculations can provide atomistic details of the atomic and electronic structures of the material and make accurate predictions of their properties. Yet, ab initio calculations of e-d interactions are still in their infancy, mainly because they require large simulation cells and computationally expensive workflows.

This talk aims to overcome the open challenges of computing the e-d interactions and the associated e-d matrix elements, e-d relaxation times, and defect-limited mobility using first-principles methods. We develop an efficient first-principles method to compute the e-d matrix elements and apply it to neutral and charged defects in silicon. We show for the first time fully ab initio calculations of the temperature-dependent defect-limited carrier mobility, which includes both electron-phonon and e-d interactions within the same framework, and investigate its numerical convergence. In summary, our methods have laid a solid foundation for future ab initio e-d interaction calculations, which can be applied broadly to address materials design challenges in electronics, energy, and quantum technologies. Near the end of the talk, I will discuss a few topics that I would like to explore in the group after I join the group in July.