Winter 2025 Joint Colloquium
Materials Department & Materials Research Laboratory

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11:00 am | ESB 1001

Advances in Ab Initio Approaches for Predicting the Nature and Fate of Photoexcitations in Emerging Semiconductors

The ability to synthesize and probe new classes of functional photoactive materials with tunable structure and composition – such as halide perovskites, transition metal oxides and nitrides, van der Waals heterostructures, organic solids, and more – has driven the development of new theory, computational methods, and intuition for predicting their photophysics. In these emerging classes of semiconductors, the behavior of photoexcitations can deviate from simple models, and new understanding is needed to interpret and predict their nature and kinetics. Here, I will discuss recent advances of ab initio approaches – computational methods based on density functional theory and many-electron Green's function formalisms – for predicting spectroscopic properties of complex materials, focusing our own recent developments that allow computation of how excitons are influenced by chemical composition, lattice structure and dynamics, temperature, dielectric screening, and carrier concentration. I will discuss the application of these new ab initio methods to several novel semiconductors, resulting in quantitative prediction of the temperature-dependence of exciton binding energies, and of exciton-exciton scattering and exciton dissociation timescales. I will close with a discussion of implications for experiments and for future computational studies of exciton dynamics in materials.

Hosted by Ram Seshadri