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Excited States and Optical Spectra Based on GW-BSE: Dimensionality and Screening[1]

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In this talk, I discuss some recent developments and applications of first-principles GW plus Bethe Salpeter equation (GW-BSE) approach to the understanding and prediction of photo-excited states, optical responses, and related spectroscopic properties of materials, in particular atomically thin two-dimensional (2D) crystals. Owing to their reduced dimensionality, quasi-2D materials and their nanostructures can exhibit highly unusual behaviors. Symmetry, many-body interactions, doping, and substrate screening effects play a critical role in shaping qualitatively and quantitatively their excited-state properties. Accurate treatment of these effects, in particular many-electron interactions, poses new theoretical and computational challenges. I will present some new developments in addressing these challenges, and present studies on monolayer and few-layer transition metal dichalcogenides and metal monochalcogenides, as well as black phosphorus and other 2D crystals. Several highly interesting and unexpected phenomena are discovered: unusual excitonic level structures and optical selection rules; exchange-induced light-like (massless) exciton dispersion in 2D; tunable optical and plasmonic properties; and the dominant influence of substrate screening.

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