Real-time approach to optical properties of 2D materials: time-dependent Bethe-Salpeter Equation

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The exciton, an electron-hole (e-h) quasiparticle has an important role in applied physics, especially for 2D materials where its binding energy is high. This peculiar effect determines the stability and localization of excitons that can be exploited either for qubits or, by using self-trapping effects, for Single Light Emitter devices. Another effect of current interest is non-linear harmonic generation in 2D materials where it can be used to extract important information regarding, e.g., the number of layers and crystallographic orientation of few-layered MoS2.

In this talk, we review that current state of art of \textit{ab initio} many-body perturbation theory, the Bethe-Salpeter Equation in the linear regime and we describe a theoretical approach (Time-dependent Bethe-Salpeter Equation) to study the nonlinear optical response of electronic systems based on a real-time solution of the electronic dynamics in the presence of time-dependent electromagnetic fields. Using accurately parameterized tight-binding models and electronic interactions, this allows expedited and accurate calculations of the nonlinear response to arbitrary order for realistic systems. We demonstrate its capabilities by computing the excitonic spectrum and high-harmonic generation (SHG, THG, FHG) in MoS2 and BN monolayers.

Host: Justin Song