Band Gap, Excitons, Thermal Conductance, and Energy Applications of Few-Layer Black Phosphorus

LI YANG, Physics Department, Washington University — I will present our recent works of the electronic structures, optical excitations, and thermal conductance of a class of newly emerging two-dimensional semiconductors, few-layer black phosphorus (phosphorene). Using first-principles calculations and models, we study several fundamental properties of few-layer black phosphorus. We predict the quasiparticle band gap, excitonic effects, and anisotropic optical spectra, which have been confirmed by recent experiments. Moreover, we predict that not only the electrical conductance but also the lattice thermal conductance is anisotropic, making this material a promising candidate for thermoelectric applications.