MAR17-2016-030205

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Many-Body Effects on the Electronic and Optical Properties of Quasi-2D Semiconductors

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Quasi-two-dimensional (quasi-2D) semiconductors are the subject of intense research interest as platforms for both developing atomically thin devices and exploring novel physics. These are layered materials with covalent bonding in each layer and weak coupling between layers so that individual layers can be easily peeled off. Changes to confinement and screening in reduced dimensions can lead to drastic changes in quasiparticle (QP) and optical properties when compared with bulk materials. We use the GW and GW-BSE methods to explain and predict the QP and optical properties of quasi-2D semiconductors. We find that quasi-2D materials have diverse, strongly-bound excitons including some with unusual (massless) dispersion. Moreover, we explore the effects of the screening environment on the QP and excitonic properties and find that encapsulation and substrate engineering can tune the QP gap and exciton binding energies by an order of magnitude. This sensitivity allows us to treat screening and confinement as separate degrees of freedom, opening new pathways for engineering the properties of low-dimensional materials.

I would like to acknowledge collaborations with members of the Louie group. This work was supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences Engineering Division, and by National Science Foundation.