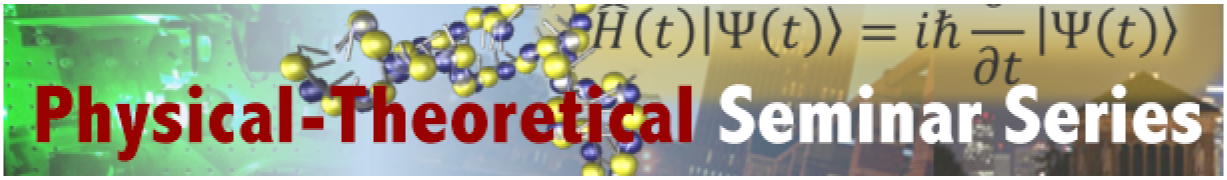

Physical-Theoretical Seminar Series

Monday, November 8, 2021
Seaver Science Library, SSL 202 (12 pm)
Broadcasting: https://usc.zoom.us/j/99398094546
Student meeting: SSC 604, 5pm

Professor Sahar Sharifzadeh

Department of Electrical and Computer Engineering
Boston University

Excitonic Properties of Imperfect 2D Materials: The Impact of Defects and Temperature from First Principles

Stable two-dimensional materials are promising for nanoelectronics due to their relatively small form factor and great variety in chemical and electronic structure, allowing for the design of light-weight and low-cost materials for optoelectronic devices such as transistors, solar cells, and lasers. We utilize first-principles theory to investigate the optoelectronic function of a series of monolayer materials, emphasizing the role of defects and electron-phonon interactions; two phenomena that will be present in and can dominate the properties of real materials, particularly in low dimensional systems with reduced screening. We utilize first-principles density functional theory (DFT) and many-body perturbation theory (MBPT) to describe excited state transitions. To describe the role of phonons, we apply the recently developed special displacement method that describes the effective exciton-phonon interaction at a given temperature from the Willams-Lax theory. For monolayer GeSe, a promising material for photocatalysis, MBPT calculations predict that the presence of a point defect results in localized mid-gap states and spatially confined excited states that can be described as localized Wannier-Mott excitons. With the inclusion of phonons, the optical absorption spectrum of pristine GeSe is red-shifted by ~ 0.1 eV, with both acoustic and optical phonons coupling to the excitonic state. To better understand the role of exciton-phonon interactions in low dimensions, we study the band gap renormalization for a series of 2D materials. We show that the strength of electron-phonon interactions is highly dependent on the bonding structure. Overall, the framework we develop allows for a systematic systematical theoretical exploration of the optoelectronic properties of materials.

Suggested reading:

1. T.A. Huang, M. Zacharias, D.K. Lewis, F. Giustino, and S. Sharifzadeh, "Exciton-Phonon Interactions in Monolayer Germanium Selenide from First-Principles," *J. Physical Chemistry Letters* **12**, 3802 (2021). https://pubs.acs.org/doi/abs/10.1021/acs.jpclett.1c00264
2. A. Cohen, D. K. Lewis, T. Huang, S. Sharifzadeh, "Localized Excitons in Defective Monolayer Germanium Selenide," *Physical Review Materials* **4**, 076002 (2020). https://journals.aps.org/prmaterials/abstract/10.1103/PhysRevMaterials.4.076002

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Hosted by Professor Oleg Prezhdo

The scientific community is invited