

Tuning the Optical Properties of 2D Materials with Defects and Strain

Chia-Hao Lee¹, Yichao Zhang¹, M. Abir Hossain², Yue Zhang², Arend M. van der Zande² and Pinshane Y. Huang^{1*}

¹ Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, United States.

² Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, United States.

* Corresponding author: pyhuang@illinois.edu

The optical properties of 2D materials can be strongly tuned by individual atomic defects such as dopants, vacancies, and grain boundaries as well as lattice strain. As a result, reliably and rapidly characterizing these features is a critical step to controllably synthesizing materials and designing devices for 2D nanoelectronics. Here, a major challenge is the large gap in length scales between the atomic-scale defects and picometer-scale strains that modulate the electronic structure of 2D systems and the 100s of nm spatial resolution of diffraction-limited optical spectroscopies. Here, we will discuss several approaches to bridge this seven-orders-of-magnitude gap in length scales in order to understand the key factors that tune the band structure, optical absorption, and photoluminescence (PL) in 2D semiconductors. Our approach utilizes multiple electron microscopy techniques, including aberration-corrected scanning transmission electron microscopy (STEM), 4D-STEM, and diffraction-filtered dark-field TEM (DF-TEM) as a method to bridge the relevant length scales and enable direct correlations with ex-situ optical spectroscopies [1,2]. We illustrate our approach on 2D transition metal dichalcogenides including WSe₂ and MoS₂, where we show that the complex PL distributions observed through large-area exfoliation can be attributed to spatial variations in the defect density of the source crystal. We also demonstrate techniques to spatially control the exciton energy by patterning the strain distribution of the crystals in two dimensions. These methods should be useful for improving reliability and control in 2D optoelectronics.

References:

[1] CH Lee et al., *Nano Letters* **20** (2020), p 3369.

[2] AM van der Zande et al., *Nature Materials* **12** (2013), p 554.

[3] The authors acknowledge funding from the DOE through award number DE-SC0020190 and the National Science Foundation's MRSEC program through grant number DMR-1720633. This work utilizes the iMRSEC shared research facilities and UIUC's Materials Research Laboratory Shared Facilities.