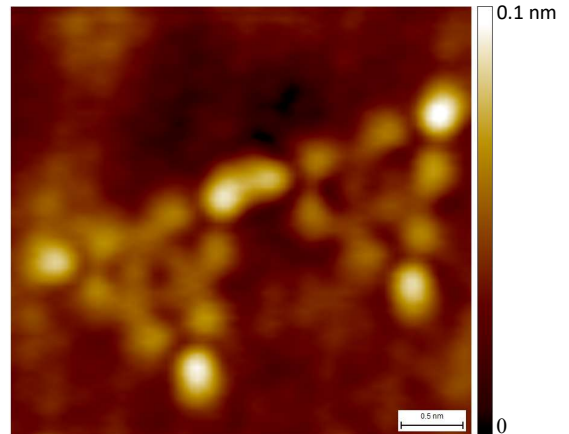


Structure and Electronic Properties Investigation of Two-Dimensional Materials**Fazel Baniasadi¹, Chenggang Tao²**¹Department of Materials Science and Engineering, Virginia Tech²Department of Physics, Virginia Tech**Abstract**

Other than graphene, two dimensional (2D) materials include transition-metal dichalcogenides (TMDCs) and trichalcogenides (TMTCs) with general formulas of MX_2 and MX_3 respectively, where M is transition metal elements (groups 4-10) and X is chalcogen elements (S, Se or Te), are two groups of 2D materials which have been extensively studied in the past few years. Also, recently 2D transition metal carbides and nitrides (Maxene) have attracted researcher's attention due to their high conductivity and stability in air giving them a very high potential for electronics and optoelectronics application.

We investigated intrinsic point defects for ultrathin 1T-PtSe₂ layers grown on mica through CVT method, using scanning tunneling microscopy and spectroscopy (STM/STS) and first-principles calculations (DFT). Point defects were formed in the structure of 1T-PtSe₂ during the growth process. Through STM/STS, we identified five types of dominant point defects and obtained their atomic structures and local density of states. We determined characteristics and formation energies of the defects using density-functional theory (DFT). The identified five defect types are Pt vacancies at the topmost and next monolayers, Se vacancies at top and bottom atomic layers in the topmost monolayer, and Se antisites at Pt sites within the topmost monolayer. Besides these all, we investigated the combination of these defects, the possibility of their existence in the structure, and how any defect combinations can influence the structure and electronic properties of the material.

**Biography**

Fazel is a fourth year PhD student currently working with Dr. Chenggang Tao. His research is to study of the structure of two dimensional (2D) materials and the behavior of defects in their structures using scanning tunneling microscopy and Spectroscopy (STM/STS). His work is mostly defect characterization and investigation of the effect of defects on electronic properties of 2D materials. He has published 9 journal papers so far. He received his bachelor's and master's degrees from Sharif University of Technology in Iran and he is expecting to graduate in Spring 2020.

