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Intrinsic Point Defects in Two Dimensional Materials

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Abstract

Transition-metal dichalcogenides (TMDs) with a general formula of MX₂, where M as transition metal elements (groups 4-10) and X as chalcogen elements (S, Se or Te), are a family of two-dimensional (2D) materials which have been extensively studied in the past few years. Defects are ubiquitous in 2D TMDs. Some defects appear from growth or annealing processes, whereas some other defects are naturally or intentionally brought into the structure during investigation, such as point defects in 2D 2H-MoS₂. Typical zero-dimensional or point defects constitute vacancies, antisites, adatoms, intercalations, interstitial dopants, and substitutional dopants. Properties of 2D TMDs are very sensitive to defects, especially for 2D semimetals and semiconductors. Depending on the properties of interest and desirable applications, defects can be beneficial or detrimental.

We investigated intrinsic point defects for ultrathin 1T-PtSe₂ layers grown on mica through CVT method,

by using scanning tunneling microscopy and spectroscopy (STM/STS) and first-principles calculations. 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 by 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.



0.15 nm

Biography

Fazel is a second year PhD student currently working with Dr. Chenggang Tao. His research is the study of defects behavior in two dimensional (2D) materials using scanning tunneling microscopy (STM). His work is mostly defect characterization and investigation of the effect of them on the electronic properties of 2D materials. He has published 5 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 2020.

