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STM study on the surface structures and defects of SnSe[1] JUNGDAE KIM, GANBAT DUVJIR, TRINH THI LY, Univ of Ulsan, TAEWON MIN, Pusan National Univ, TAEHOON KIM, SANG HWA KIM, ANH-TUAN DUONG, S. H. RHIM, SUNGLAE CHO, Univ of Ulsan, JAEKWANG LEE, Pusan National Univ — Tin selenide (SnSe) is a IV-VI semiconductor with a band gap of 1.0 eV, and also one of layered chalcogenide materials (LCMs) where each layer is coupled by weak van der Waals interactions. SnSe has been widely studied due to its many potential applications that take advantage of its excellent thermoelectric, photovoltaic, and optoelectronic properties. However, experimental investigations into the microscopic structure of SnSe remain largely unexplored. The atomic and electronic structures of SnSe surfaces are studied by a home-built low temperature scanning tunneling microscope (STM). The cleaved surface of SnSe is comprised of covalently bonded Se and Sn atoms in zigzag patterns. However, rectangular periodicity was observed in the atomic images of SnSe surfaces for filled and empty state probing. Detailed atomic structures are analyzed by density functional theory (DFT) calculations, indicating that the bright extrusions of both filled and empty state images are mostly located at the positions of Sn atoms. We also report the origin of p-type behavior in SnSe by investigating three dominant intrinsic defects (Sn, Se, and Se-Sn-Se vacancies) using STM and DFT calculations.

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