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New-class of Semiconducting 2D materials: Tin Dichalcogenides (SnX₂) CAN ATACA, Department of Materials Science and Engineering, Massachusetts Institute of Technology, KEDI WU, School for Engineering of Matter, Transport and Energy, Arizona State University, KAYAHAN SARITAS, Department of Materials Science and Engineering, Massachusetts Institute of Technology, SEFAATTIN TONGAY, School for Engineering of Matter, Transport and Energy, Arizona State University, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Recent studies have focused on a new generation of atomically thin films of semiconducting materials. A broad family of two-dimensional (2D) semiconducting transition metal dichalcogenides (MX₂) have been fabricated and investigated in monolayer, bilayer and few layer form. In this work, we investigated the electronic, optical and elastic properties of single and few layer and bulk SnX₂ (X= S, Se) both theoretically and experimentally. Using density functional theory (DFT) we carried out stability analysis through phonon and electronic, optical and elastic structure calculations. Single-few layer SnX₂s are mechanically exfoliated and Raman and photoluminescence (PL) measurements are taken. UV-Vis absorption spectrum together with PL measurements and DFT calculations yield an indirect gap of ~ 2.5 eV for SnS₂ structures (bulk). Tunability of the energy band gap and indirect-direct gap transitions are investigated by controlling the number of layers and applied stress. Lowering the number of layers decreases the indirect gap (0.1-0.3 eV), but indirect-direct gap transition occurs when layer-layer distance is reduced. Due to flexibility in engineering the electronic and optical properties, SnX₂ compounds are promising materials for future optoelectronic nanoscale applications.

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