Electronic Supplementary Material (ESI) for Materials Advances.

Hole doping at Sn sublattice of the buckled honeycomb SnX (X = S and Se) monolayer: An effiecient functionalization approach

D. M. Hoat[1,2,*] and J. Guerrero-Sanchez[3]

[1]Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

[2]Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Viet Nam

[3]Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Apartado Postal 14, Ensenada, Baja California, Código Postal 22800, Mexico

*Corresponding author: dominhhoat@duytan.edu.vn

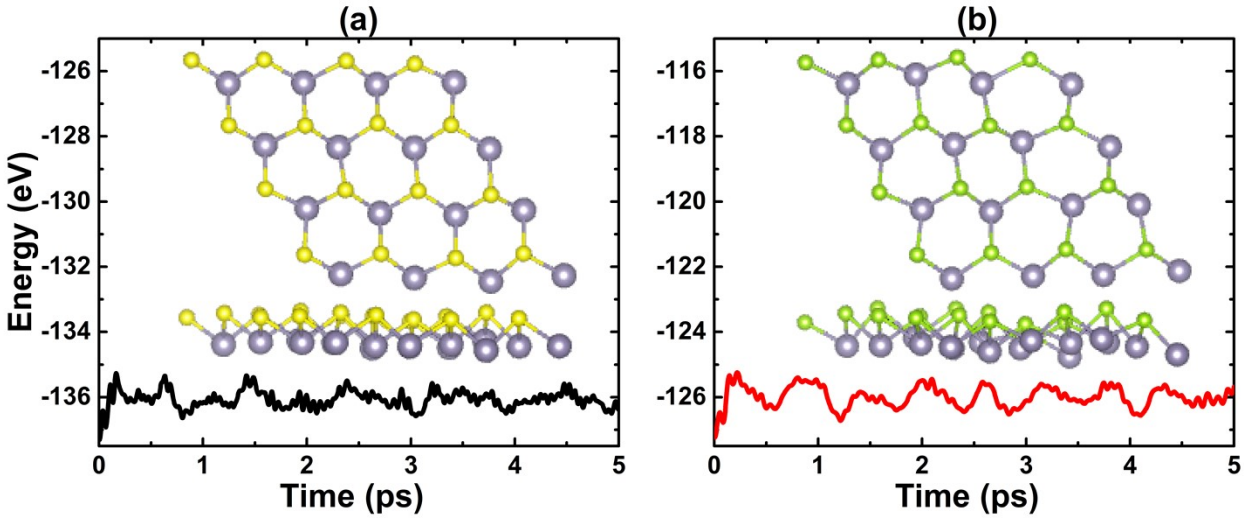

Figure S1: AIMD simulations (Energy fluctuations) at 300 K of (a) SnS and (b) SnSe monolayer (Inset: Atomic structure after 5 ps of simulations).

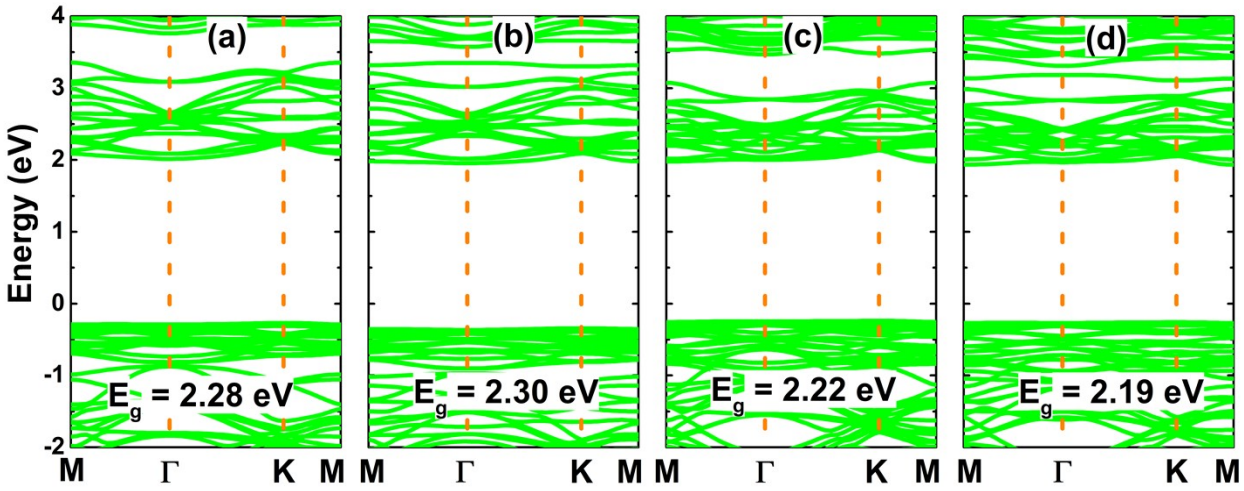

Figure S2: Electronic band structure (The Fermi level is set to 0 eV) of SnS monolayer doped with (a) Mg and (b) Ca, and SnSe monolayer doped with (c) Mg and (d) Ca.