

# Modulation of electronic and magnetic properties of defective and TM-doped Al<sub>2</sub>SSe Janus monolayer (TM = Mn and Fe) through hole and electron doping

Nguyen Thi Han,<sup>1</sup> Chu Viet Ha,<sup>2</sup> Nguyen Thanh Son,<sup>3</sup> J. Guerrero-Sanchez,<sup>4</sup> and D. M. Hoat<sup>5,6\*</sup>

<sup>1</sup>Department of Basic Science, Hung Yen University of Technology and Education, Hung Yen, Vietnam

<sup>2</sup>Faculty of Physics, TNU-University of Education, Thai Nguyen, 250000, Vietnam

<sup>3</sup>Center of Scientific Research and Application, Lac Hong University, No.10 Huynh Van Nghe Str, Tran Bien Ward, Dong Nai Province, Vietnam

<sup>4</sup>Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Apartado Postal 14, Ensenada, Baja California, Código Postal 22800, Mexico

<sup>5</sup>Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

<sup>6</sup>School of Engineering and Technology, Duy Tan University, Da Nang 550000, Viet Nam

\*Corresponding author: [dominhhoat@duytan.edu.vn](mailto:dominhhoat@duytan.edu.vn)

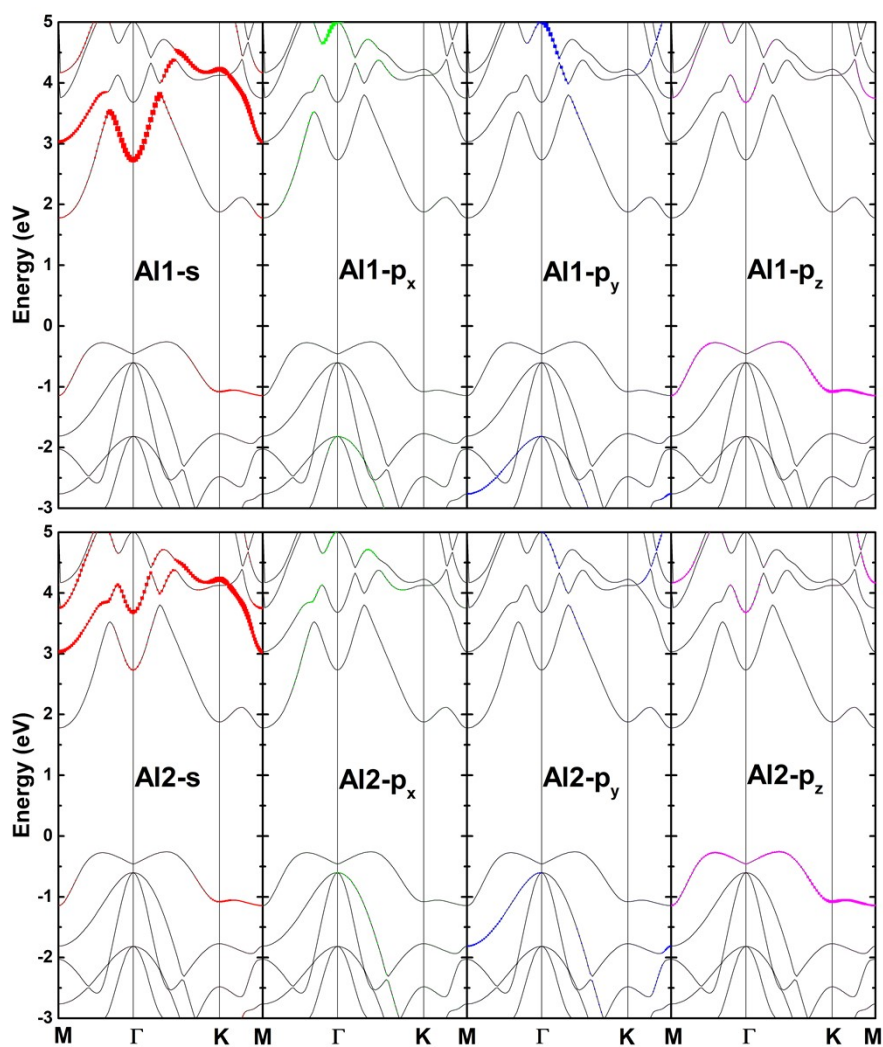


Figure S1: Orbital-decomposed band structure of  $\text{Al}_2\text{SSe}$  Janus monolayer (The Fermi level is set to 0 eV).

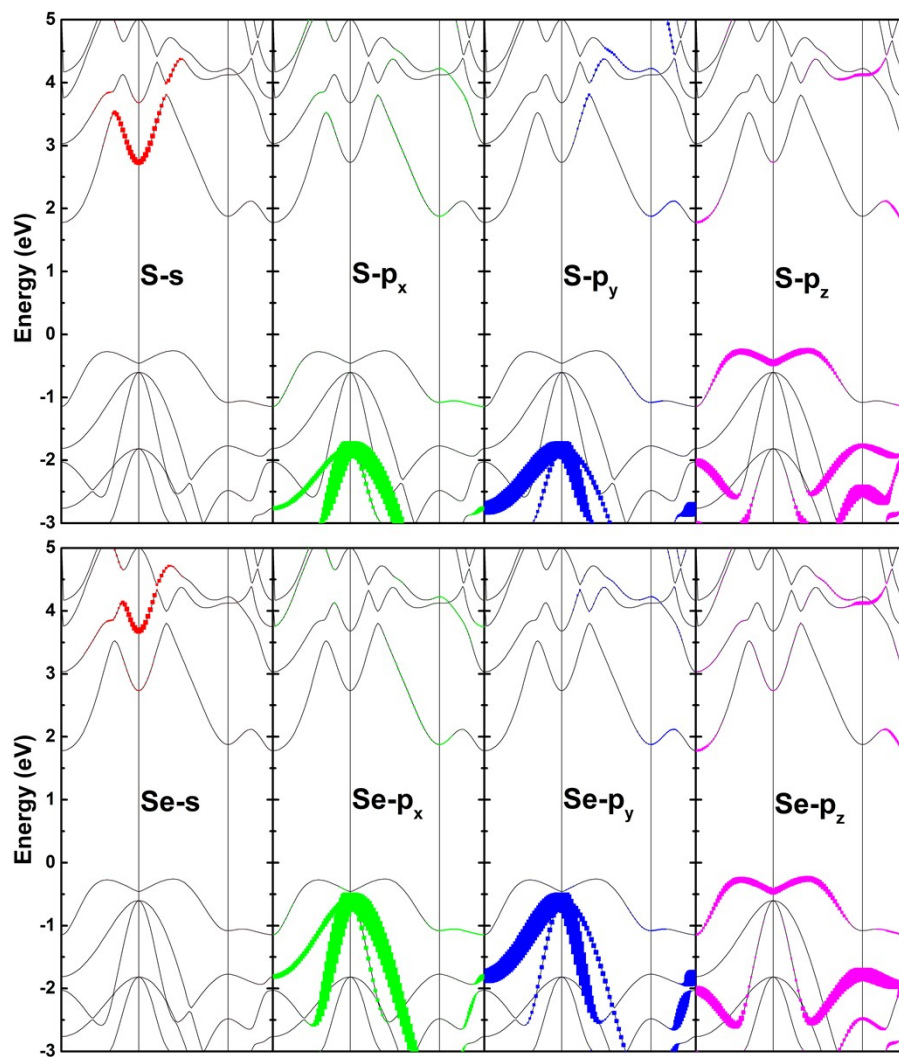


Figure S1 (cont): Orbital-decomposed band structure of  $\text{Al}_2\text{SSe}$  Janus monolayer (The Fermi level is set to 0 eV).