

Searching for d^0 spintronic materials: Bismuthene monolayer doped with IVA-group atoms

Duy Khanh Nguyen,¹ To Vinh Bao,¹ Nguyen Anh Kha,¹ R. Ponce-Pérez,² J. Guerrero-Sanchez,² and D. M. Hoat^{3,4,*}

¹High-Performance Computing Lab (HPC Lab), Information Technology Center, Thu Dau Mot University, Binh Duong Province, Vietnam

²Universidad Nacional Autónoma de México, Centro de Nanociencias y Nanotecnología, Apartado Postal 14, Ensenada, Baja California, Código Postal 22800, Mexico

³Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

⁴Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Viet Nam

*Corresponding author: dominhhoat@duytan.edu.vn

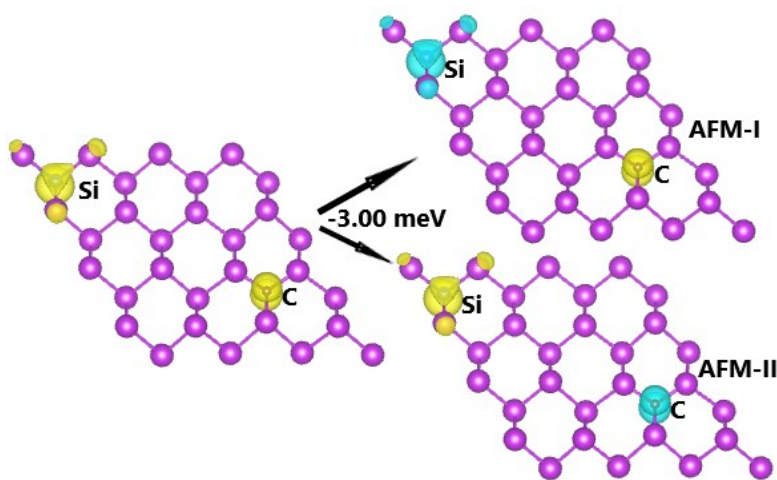


Figure S1: Spin ordering in the bismuthene monolayer co-doped with C and Si (Spin-up: yellow surface; Spin-down: cyan surface; Iso-surface value: 0.002).

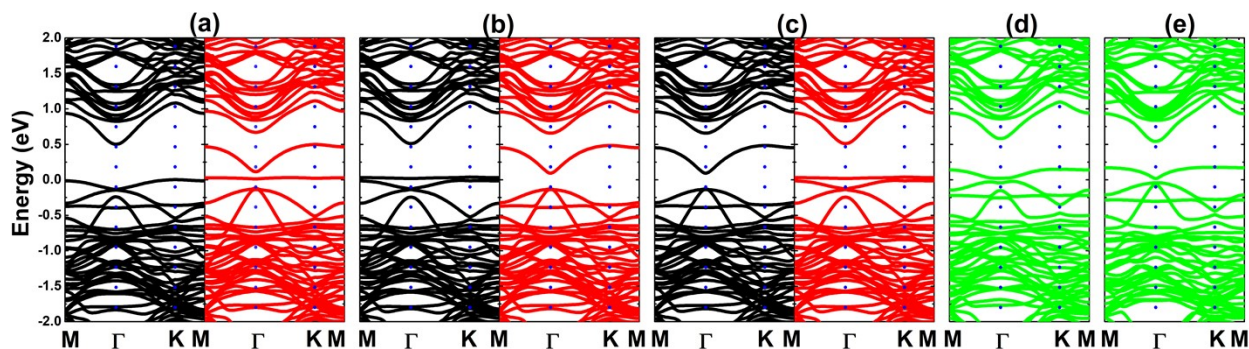


Figure.S2: Electronic band structure (Spin-up: black curve; Spin-down: red curve; Non spin-polarized: green curve; The Fermi level is set to 0 eV) of the bismuthene monolayer co-doped with (a-b-c) C and Si (a: FM, b: AFM-I, c: AFM-II), (d) C and Ge, and (e) Si and Ge

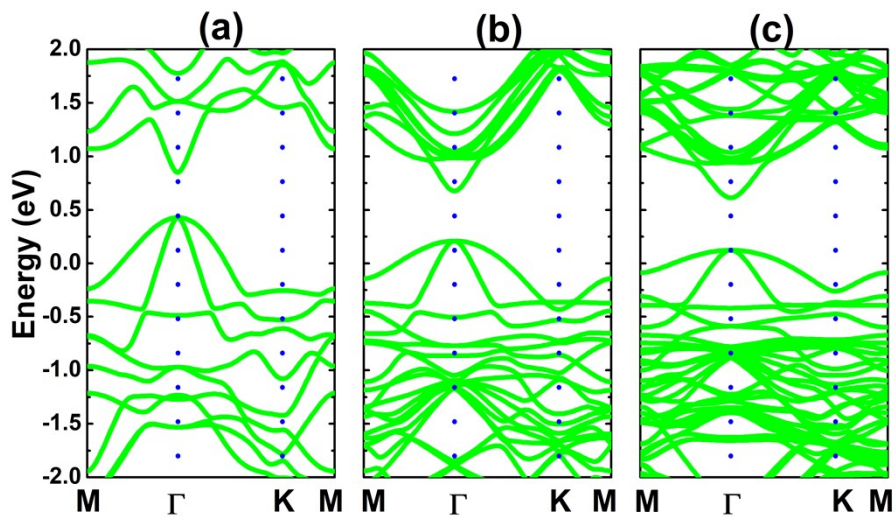


Figure 3. Electronic band structure (Non spin-polarized: green curve; The Fermi level is set to 0 eV) of the Sn-doped bismuthene monolayer with doping level of (a) 25%, (b) 11.11%, and (c) 6.25%.

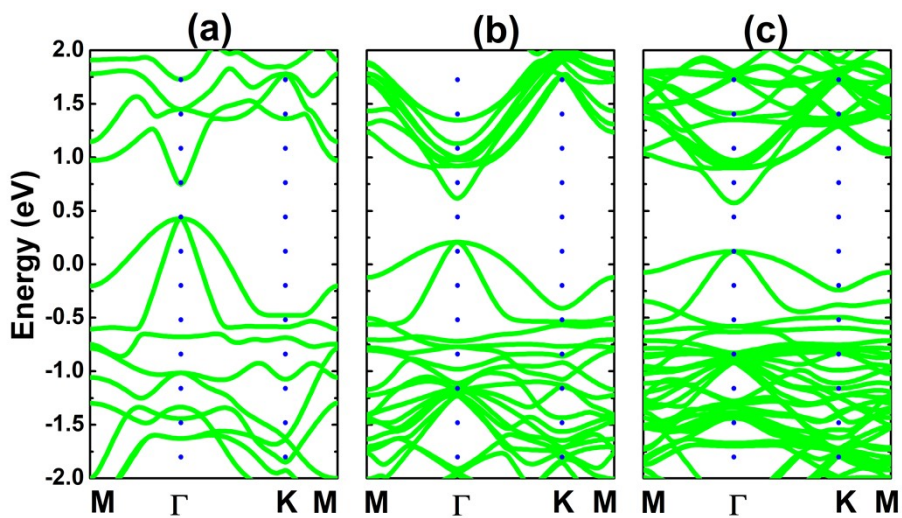


Figure 4. Electronic band structure (Non spin-polarized: green curve; The Fermi level is set to 0 eV) of the Pb-doped bismuthene monolayer with doping level of (a) 25%, (b) 11.11%, and (c) 6.25%.