

Supplementary Material

Two-dimensional Janus Semiconductors BiTeCl and BiTeBr monolayers: A first-principles study of the tunable electronic properties via electric field and mechanical strain

A. Bafekry,^{1,2,*} S. Karbasizadeh,³ C. Stampfl,⁴ M. Faraji,⁵ D. M. Hoat,^{6,7} I. Abdolhosseini Sarsari,³ S.A.H Feghi,¹ and M. Ghergherehchi^{8,†}

¹ Department of Radiation Application, Shahid Beheshti University, Tehran, Iran

² Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

³ Department of Physics, Isfahan University of Technology, Isfahan, 84156-83111, Iran

⁴ School of Physics, The University of Sydney, New South Wales 2006, Australia

⁵ Micro and Nanotechnology Graduate Program, TOBB University of Economics and Technology, Sogutozu Caddesi No 43 Sogutozu, 06560, Ankara, Turkey

⁶ Institute of Theoretical and Applied Research, Duy Tan University, Ha Noi 100000, Viet Nam

⁷ Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Viet Nam

⁸ Department of Electrical and Computer Engineering, Sungkyunkwan University, 16419 Suwon, Korea

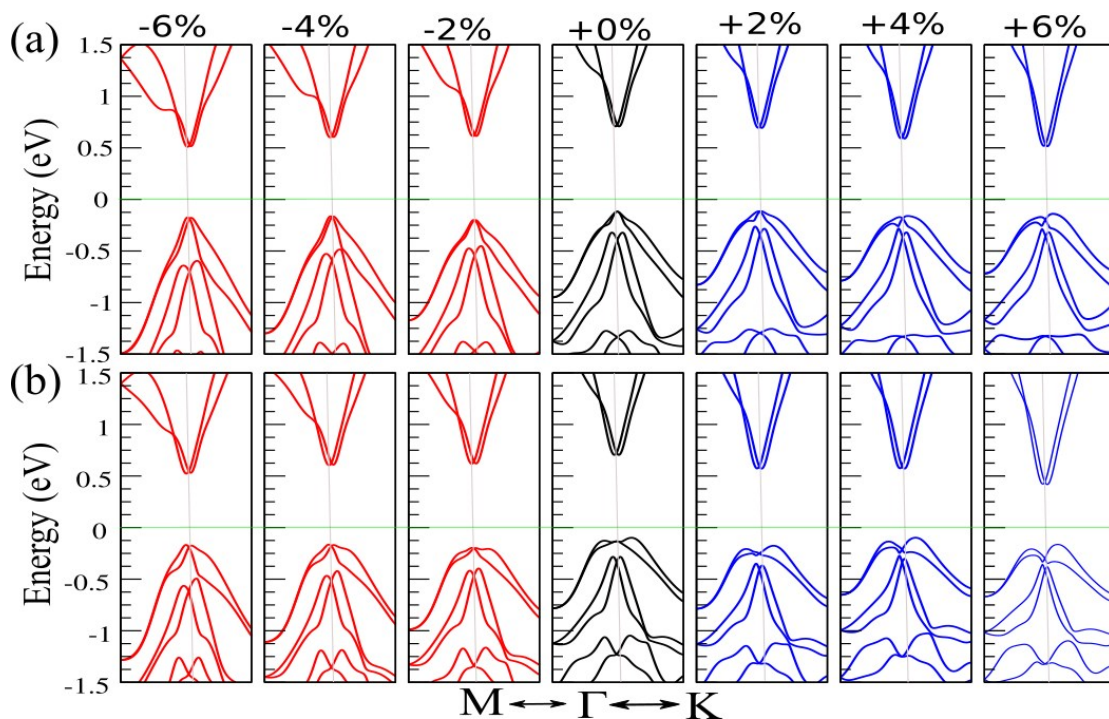


Figure S1: The electronic band structure of the BiTeCl monolayer under the influence of uniaxial strain.

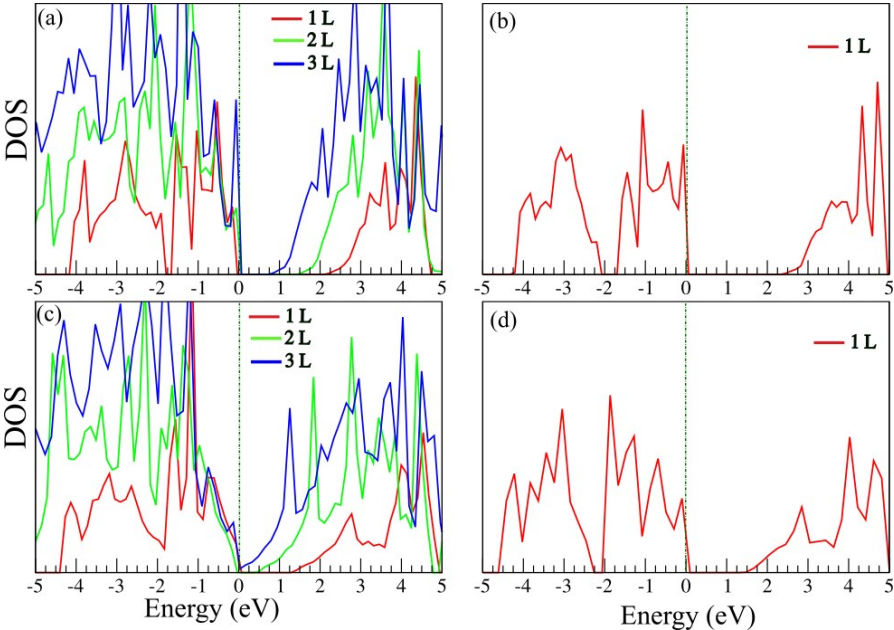


Figure S2: Electronic density of states using HSE of the (a) BiTeBr and (b) BiTeCl. Electronic density of states using HSE+SOC of (c) BiTeBr (d) BiTeCl monolayers.