

Supporting Information (SI)

First principles prediction of two-dimensional Janus

XMoGeN₂ (X = S, Se and Te) materials

Son-Tung Nguyen¹, Pham V. Cuong¹, Cuong Q. Nguyen^{2,3,†}, Chuong V. Nguyen^{4,†}

¹*Faculty of Electrical Engineering Technology, Hanoi University of Industry, Hanoi 100000, Vietnam*

²*Institute of Research and Development, Duy Tan University, Da Nang 550000, Vietnam.*

³*Faculty of Natural Sciences, Duy Tan University, Da Nang 550000, Vietnam*

⁴*Department of Materials Science and Engineering,*

Le Quy Don Technical University, Ha Noi 100000, Vietnam

[†]*Corresponding authors: chuong.vnguyen@lqdtu.edu.vn and nguyenquangcuong3@duytan.edu.vn*

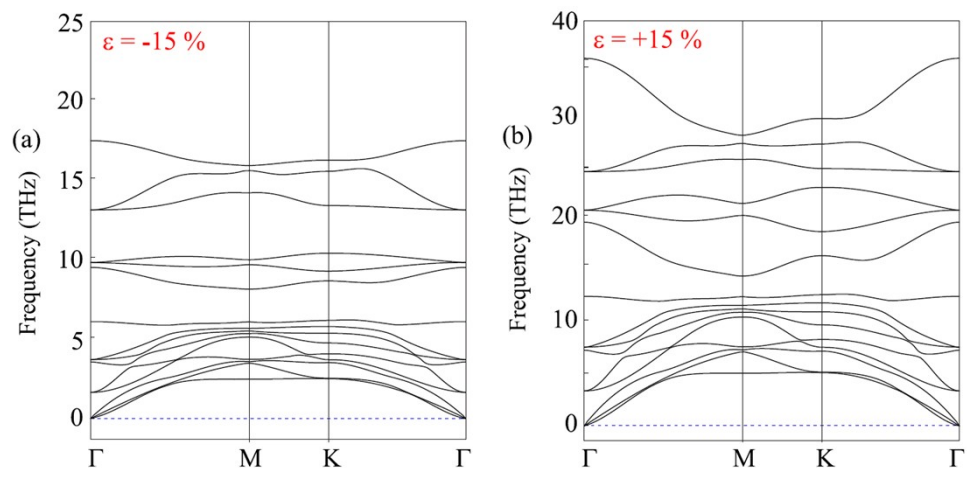


Fig. S1. Phonon spectrum of TeMoGeN2 monolayer under strain of (a) -15 % and (b) +15 %.

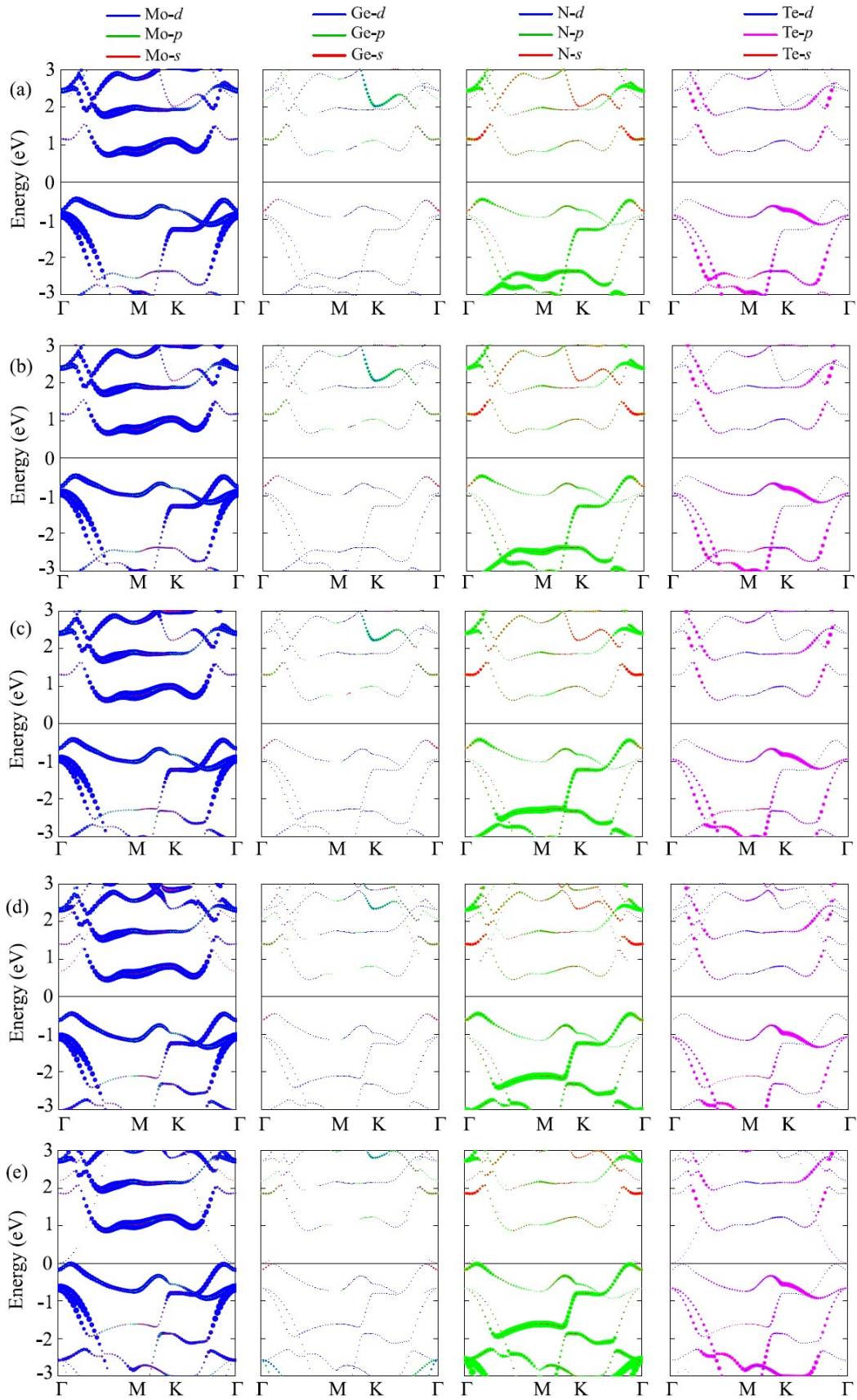


Fig. S2. Orbital projected band structures for TeMoGeN₂ monolayer under different strengths of electric field of (a) $E = -1.0$ V/nm, (b) $E = -0.7$ V/nm, (c) $E = 0$ V/nm, (d) $E = +0.7$ V/nm and (e) $E = +1.0$ V/nm.

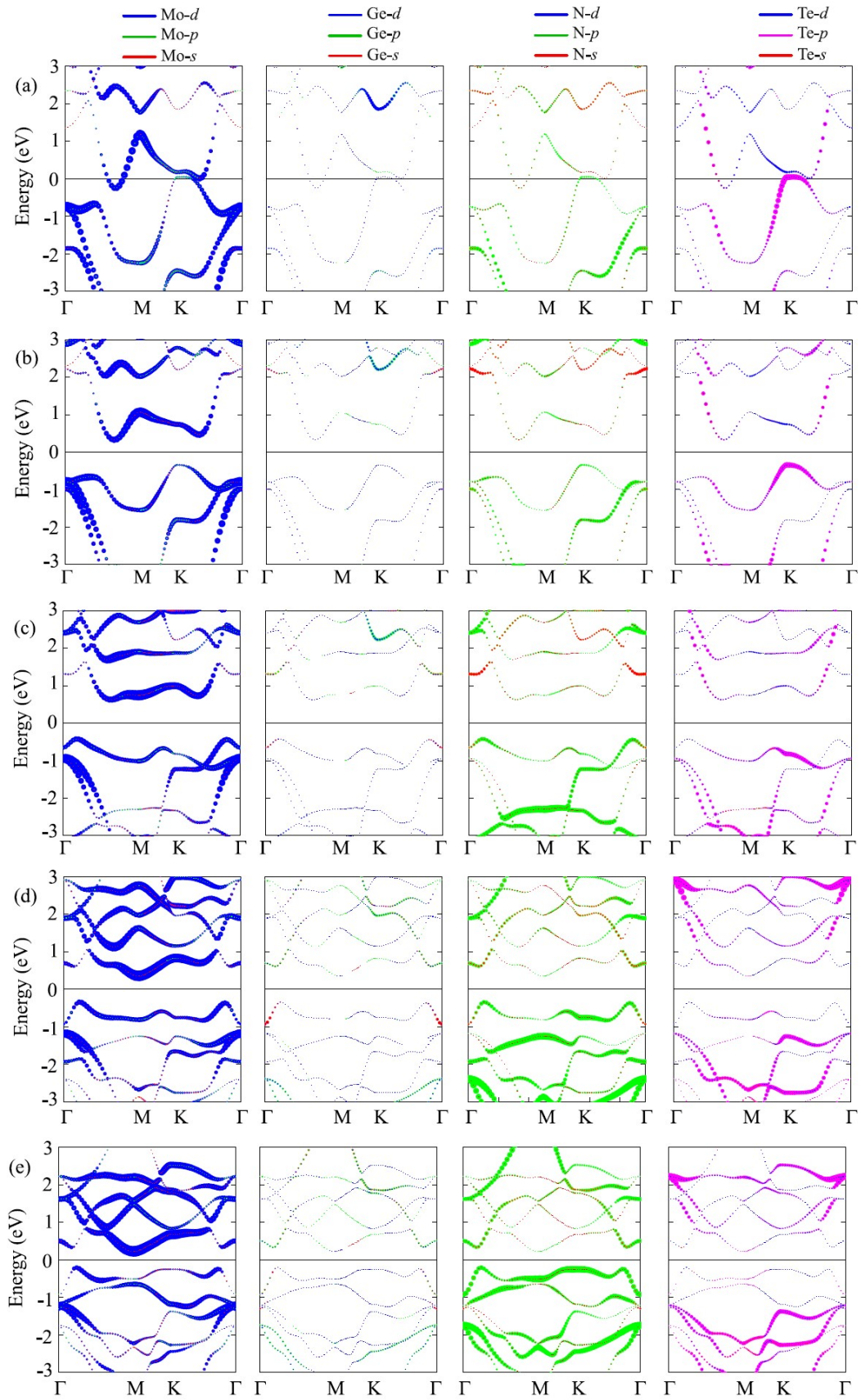


Fig. S3. Orbital projected band structures for TeMoGeN₂ monolayer under different strengths of electric field of different strains of (a) $\epsilon = -15\%$, (b) $\epsilon = -8\%$, (c) $\epsilon = 0\%$, (d) $\epsilon = +8\%$, and (e) $\epsilon = +15\%$.