Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2021

Supplementary Material for

Flexible Ferroelasticity in Monolayer PdS_2: a DFT Study

Wei Zhang, Yang Cui, Chuanhui Zhu, Biyi Huang and Shubin Yan*

College of Electrical Engineering, Zhejiang University of Water Resources and Electronic Power, Hangzhou 310018, People's Republic of China

E-mail: zhangw@zjweu.edu.cn

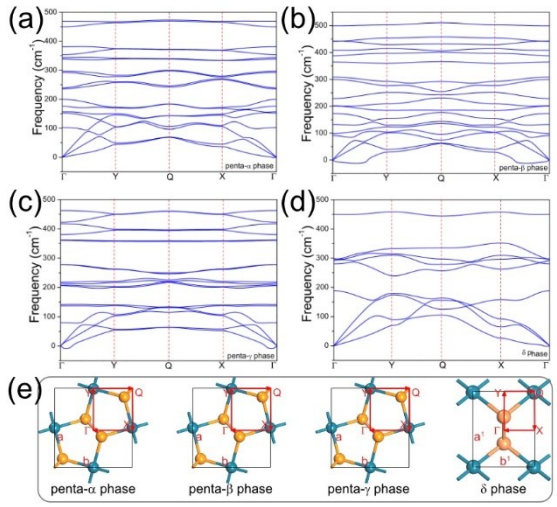

Figure s1. The phonon dispersion curves of monolayer PdS_2 in (a)penta-α phase, (b) penta-β phase, (c) penta-γ phase, and (d) δ phase. (e) The integration path in Brillouin zone used for phonon dispersion calculations including high symmetry points of Γ (0, 0, 0), Y (0, 0.5, 0), Q (0.5, 0.5, 0) and X (0.5, 0, 0).

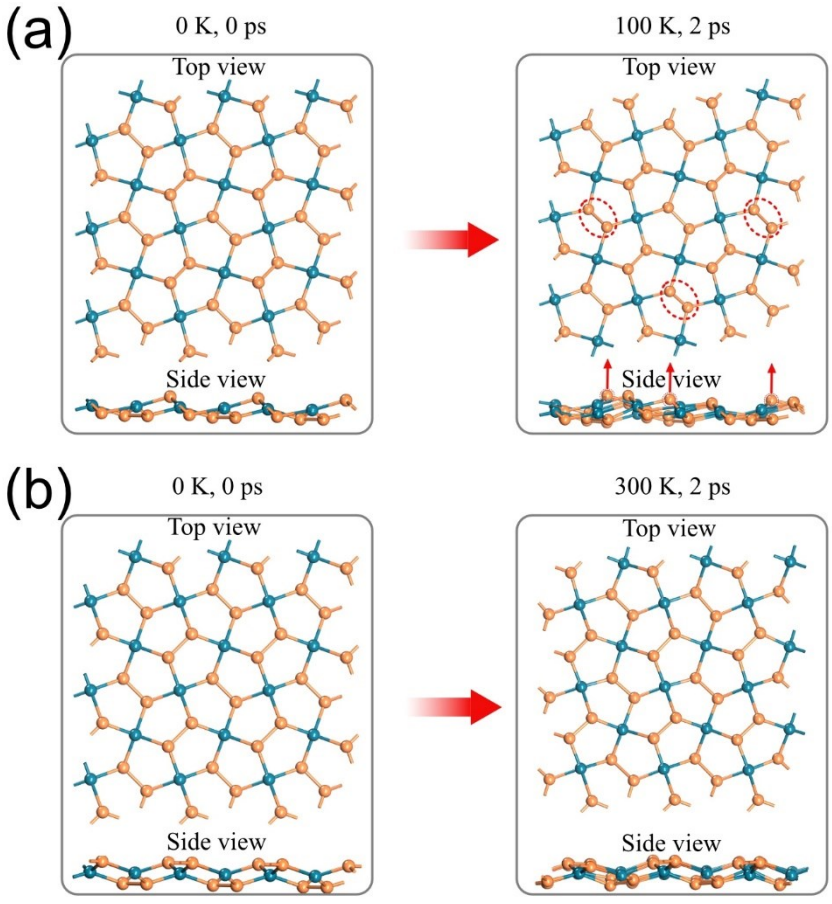

Figure s2. Top and side views of AIMD simulations for (a)penta-β and (b) penta-γ monolayer PdS_2 (supercell: 3×3×1).

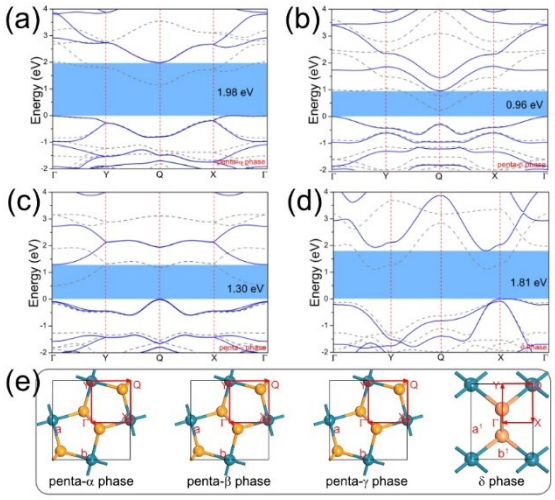

Figure s3. Calculated band structure of monolayer PdS_2 in (a)penta-α phase, (b) penta-β phase, (c) penta-γ phase, and (d) δ phase with PBE (grey dash lines) and HSE (blue lines) method. (e) The integration path in Brillouin zone used for electronic structure calculations, which includes high symmetry points of Γ (0, 0, 0), Y (0, 0.5, 0), Q (0.5, 0.5, 0) and X (0.5, 0, 0).

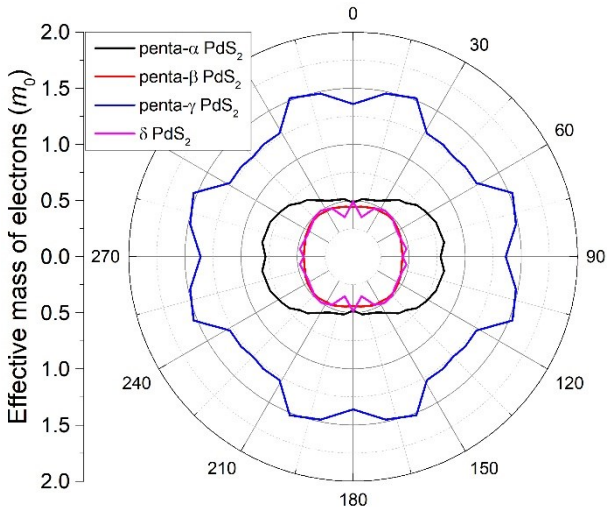

Figure s4. The effective mass of electron according to the spatial direction (0~360) for monolayer PdS_2 in penta-α phase, penta-β phase, penta-γ phase, and δ phase.

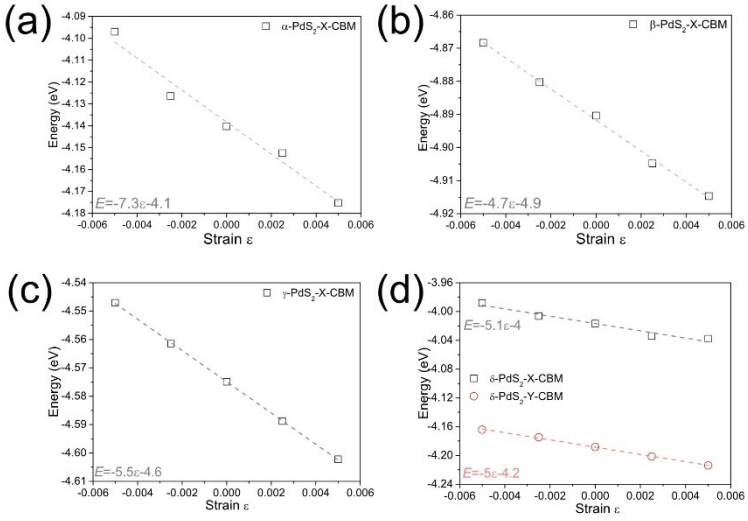

Figure s5. Energy shift of CBM for monolayer PdS_2 in (a)penta-α phase, (b) penta-β phase, (c) penta-γ phase, and (d) δ phase with respect to the lattice dilation and compression along X and Y direction, respectively.

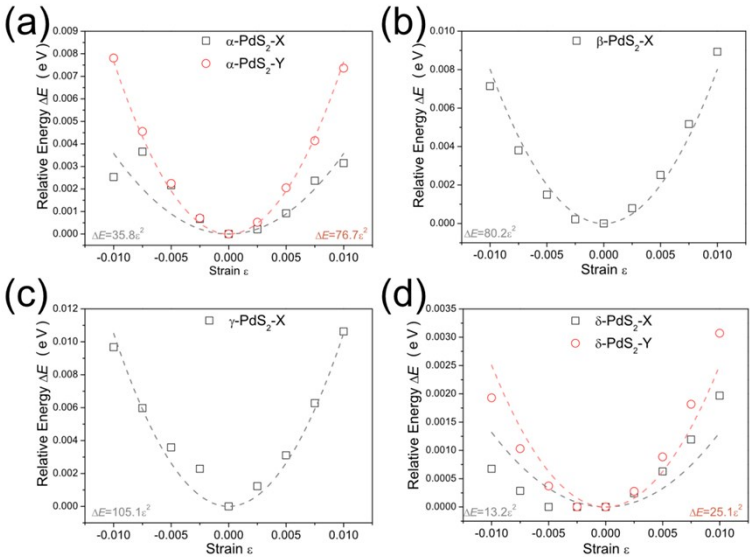

Figure s6. Energy difference between the total energy of relaxed and strained monolayer PdS_2 in (a)penta-α phase, (b) penta-β phase, (c) penta-γ phase, and (d) δ phase along X and Y directions.

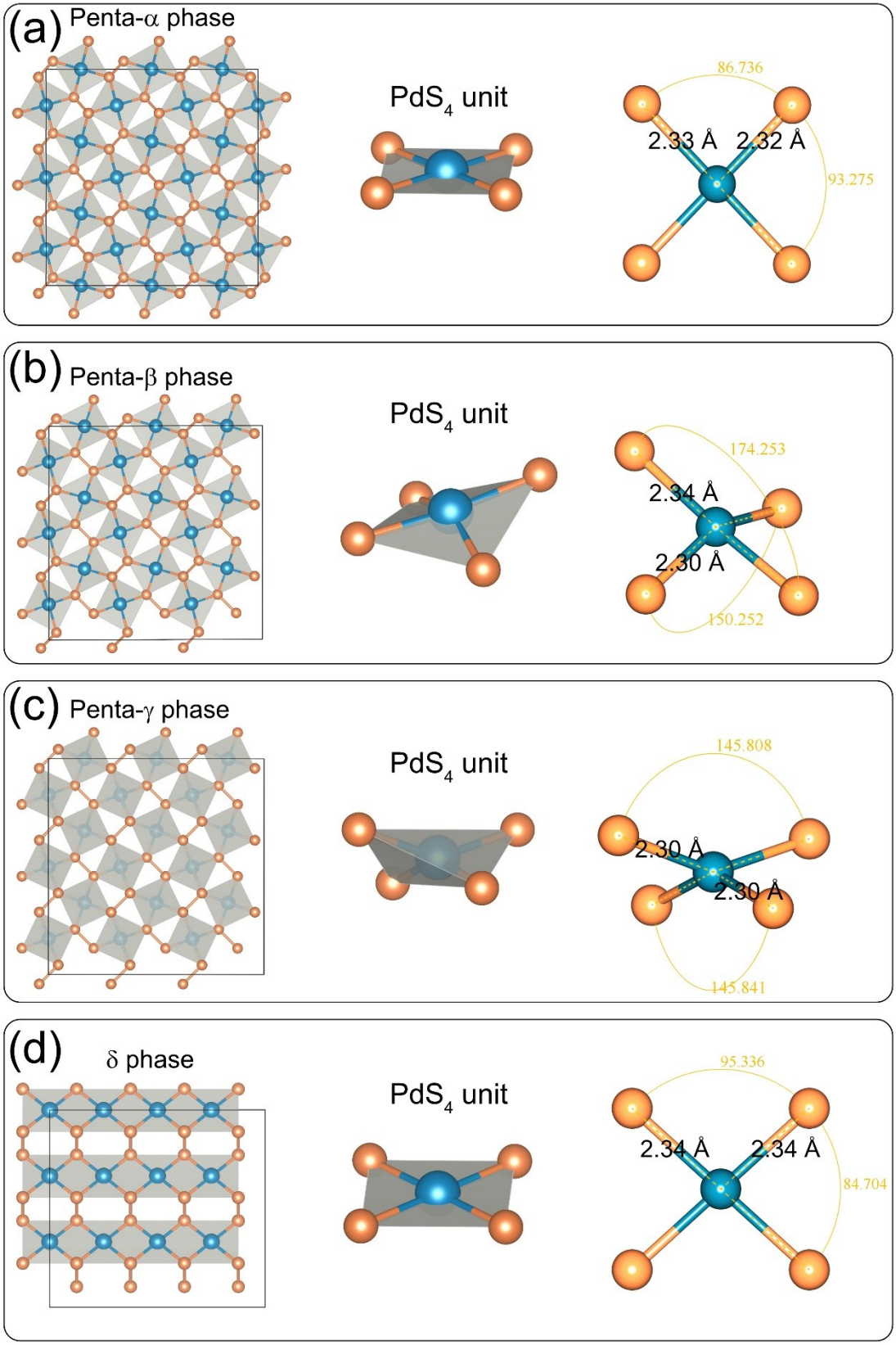

Figure s7. Top view of PdS_2 supercell in (a) penta-α, (b) penta-β, (c) penta-γ and (d) δ phases with four kinds of PdS_4 units.