Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Support Information

Table SI.

	CP-1	CP-2	CP-3	CP-4	CP-5	CP-6
D_a	0.382%	0.368%	0.175%	0.175%	0.261%	0.268%
D_{TE}	0.071%	0.068%	0.066%	0.066%	0.068%	0.067%

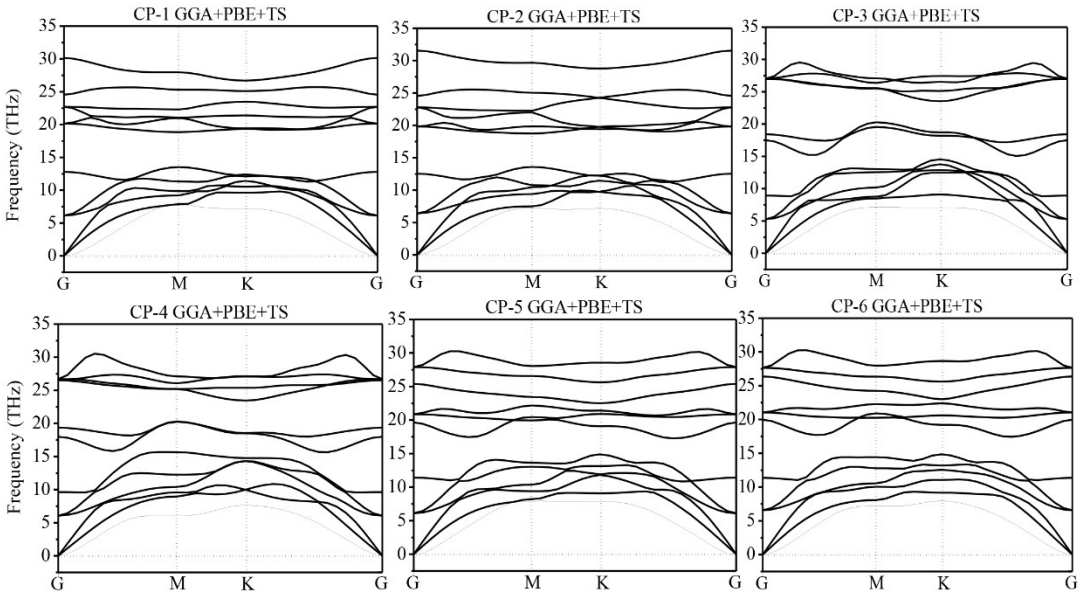

Fig. S1 (a)-(d) The phonon spectrum of all C_2P_2 monolayers with considering van der Walls dispersion correction.

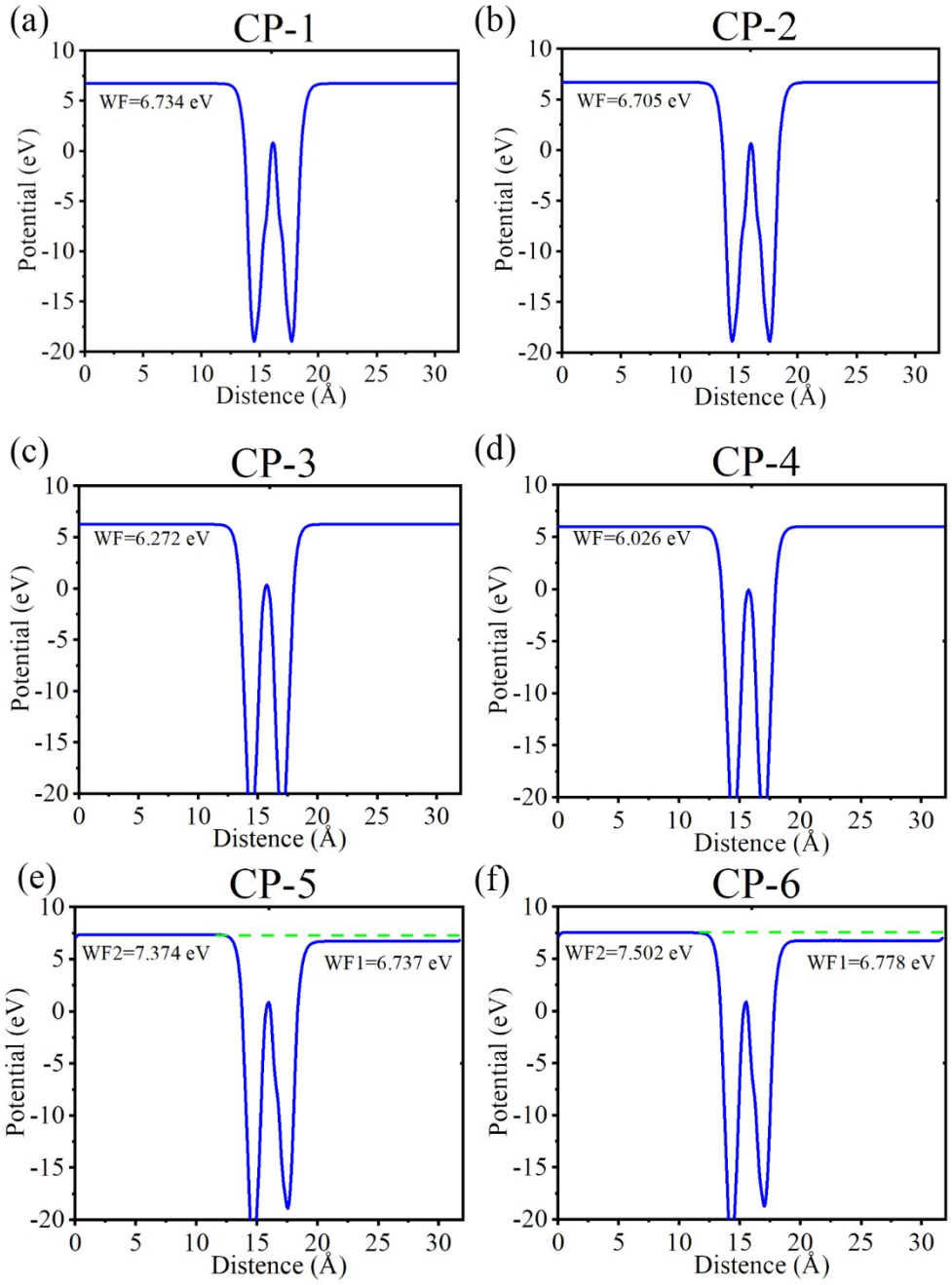

Fig. S2 (a) - (d) The Plane-averaged electrostatic potential of non-Janus C_2P_2 monolayers, where the work functions are donated as 6.734 eV, 6.705 eV, 6.272 eV and 6.026 eV, respectively. (e)-(f) The Plane-averaged electrostatic potential of Janus C_2P_2 monolayers,

Where, due to the build-in electric field of Janus C_2P_2 monolayers, the work functions of CP-5 are 7.374 and 6.737 for VBM and CBM, respectively, and the work functions of CP-6 are 7.502 and 6.778, for VBM and CBM, respectively.

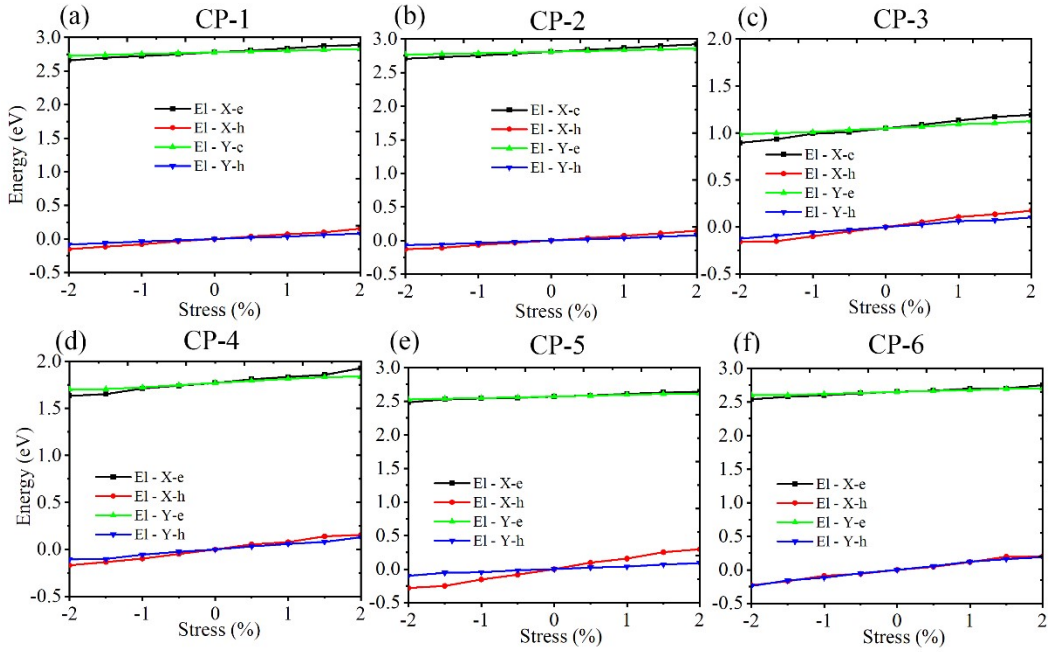

Fig. S3 (a-f) The Strain effect on the VBM and CBM of monolayer C_2P_2. The slope of linear fitting of these data represents deformation energies *El* (eV).

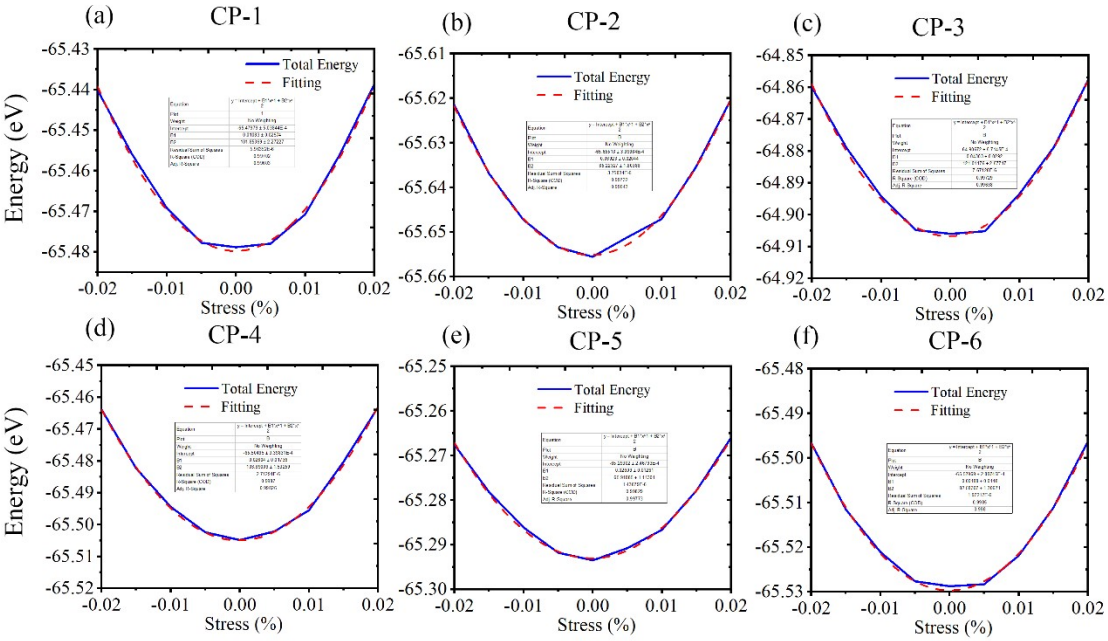

Fig. S4 (a-f) The Strain along X direction effect on total energy of monolayer C_2P_2 .

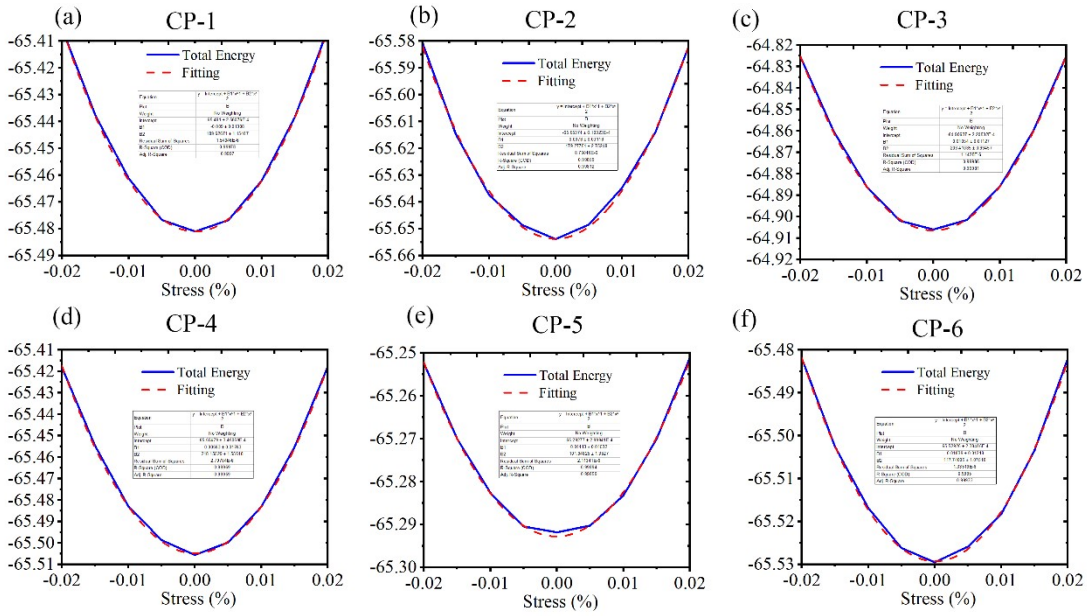

Fig. S5 (a-f) The Strain along Y direction effect on total energy of monolayer C_2P_2 .