Carbon phosphide nanosheet and nanoribbon: insights on modulating their electronic properties by first principles calculations

Tong Chen, Huili Li, Yuyuan Zhu, Desheng Liu, Guanghui Zhou, and Liang Xu

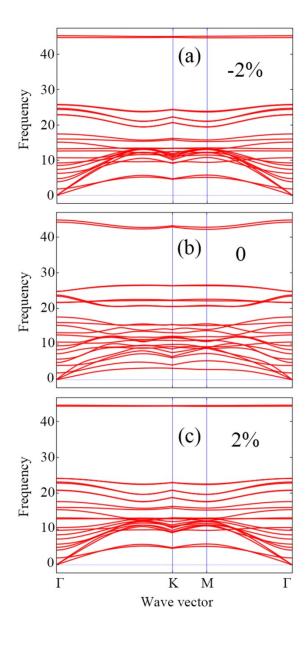


Fig. S1 (a)-(c) Phonon dispersion for 2D CP nanosheets under different strains 0f -2%, 0, +2% along the biaxial direction.

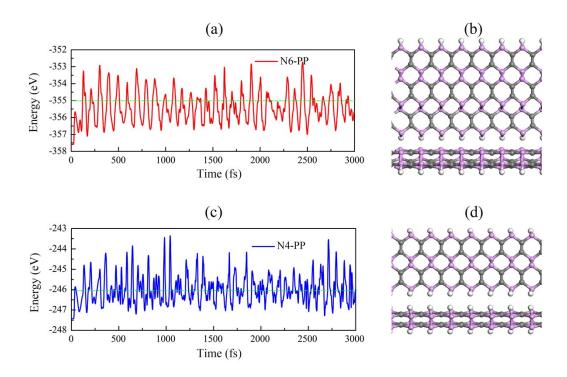


Fig. 2S (a) and (c) Variation of the free energy of N6-PP and N4-PP in the molecular dynamics simulation at room temperature during the time scale of 3.0 ps, respectively. (b) and (d) The final structures of N6-PP and N4-PP in the molecular dynamics simulation.