Supporting Information

Direction-Control of Anisotropic Electronic Behaviors via Ferroelasticity in Two-Dimensional α-MPI (M = Zr, Hf)

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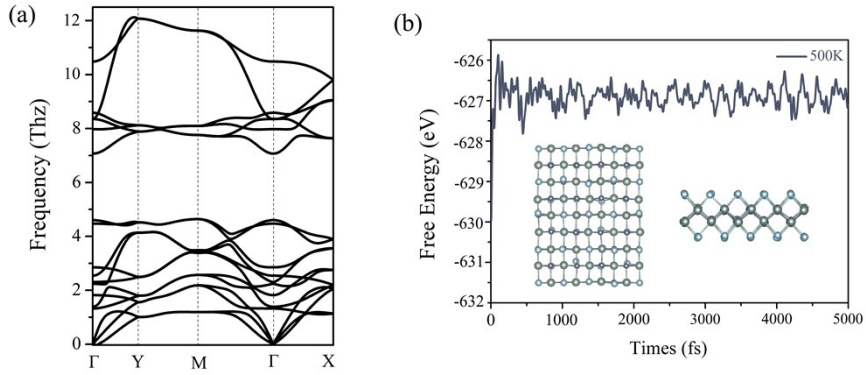

Fig. S1. (a) Phonon spectra of SL α-HfPI. (b) Variation of total energy of SL α-HfPI with time obtained from AIMD simulation at 500K. Inset in (b) is the snapshot taken from the end of the AIMD simulation.

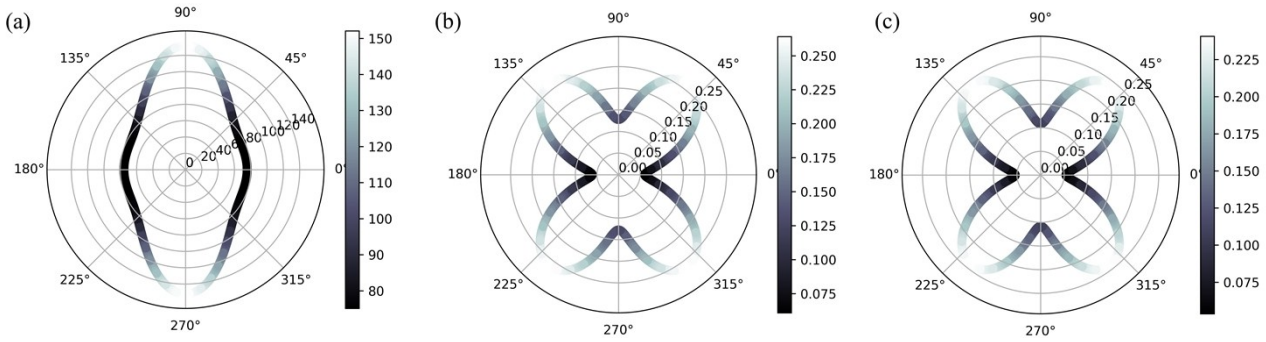

Fig. S2. (a) Young's modulus of SL α-HfPI, (b) Possion's ration of SL α-ZrPI and (c) Possion's ration of SL α-HfPI as a function of the angle θ ($\theta = 0\circ$ corresponds to the x axis).

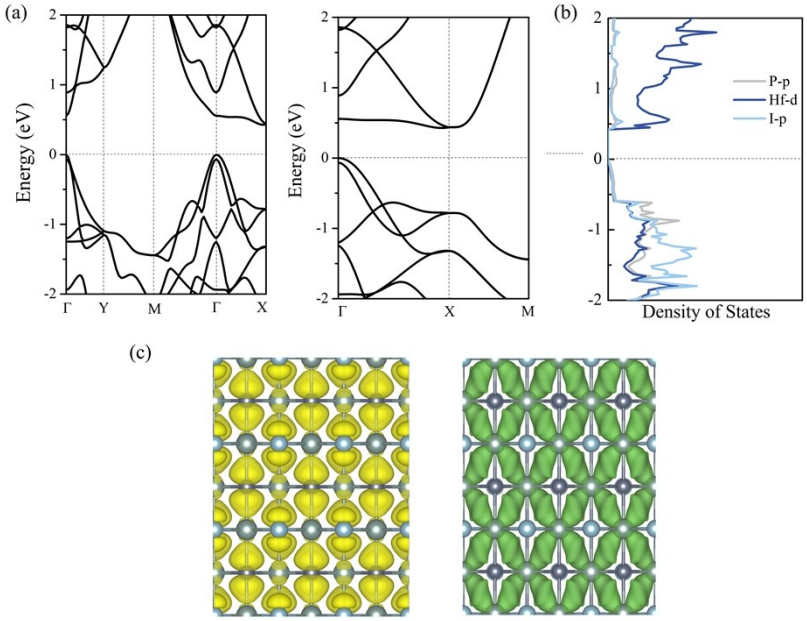

Fig. S3. (a) The band structure and (b) projected density of states of SL α-HfPI. The Fermi level is set to zero. The right panel in (a) shows the band dispersions around CBM. As shown in (a), the CBM locates around the X point instead of the Γ point. The dispersion of the bottom conduction

band along the y direction is rather flat, thus resulting in the large effective mass of electron for α-HfPI. (c) The partial charge density of VBM (left) at the Γ point and CBM (right) around the X point of SL α-HfPI.

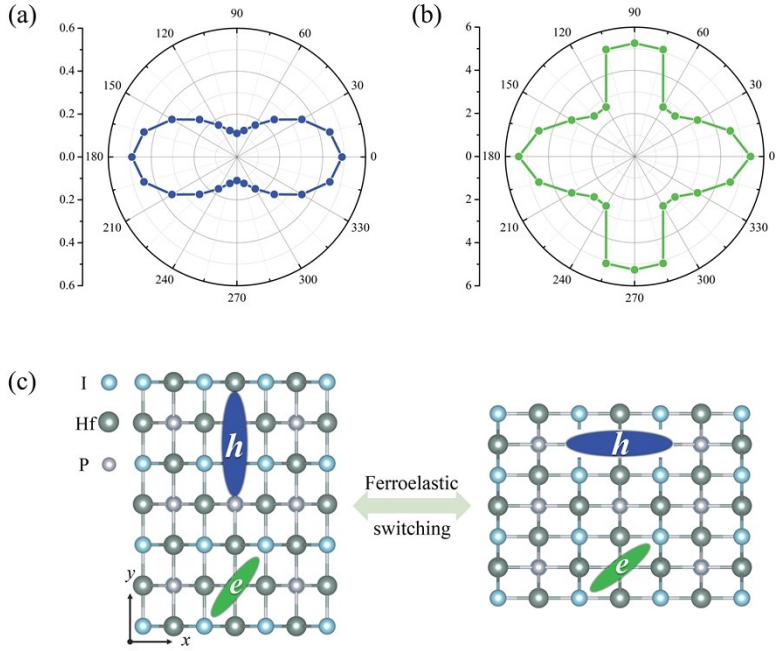

Fig. S4. The direction-dependent effective masses of (a) holes and (b) electrons for SL α-HfPI. $\theta = 0^{\circ}$ corresponds to the x axis. (c) The schematic diagram of the anisotropy of carrier transports for SL α-HfPI controlled by ferroelastic switching. According to the directional electron effective mass in Fig. S4(b), electrons of SL α-HfPI prefer to transport along Γ-M direction, rather than along x or y direction. The electron mobility along M direction is 3.24×10^{2} cm^{2} V^{-1} s^{-1}.

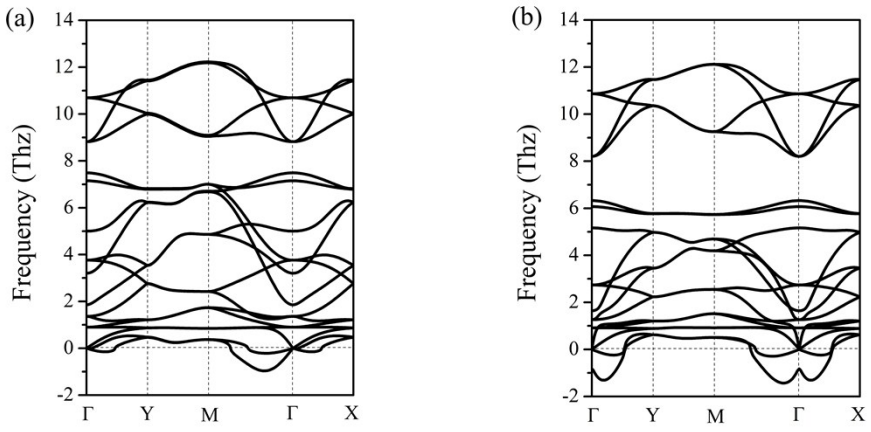

Fig. S5. Phonon spectra of (a) SL α-ZrPI and (b) SL α-HfPI with the intermediate square lattice.

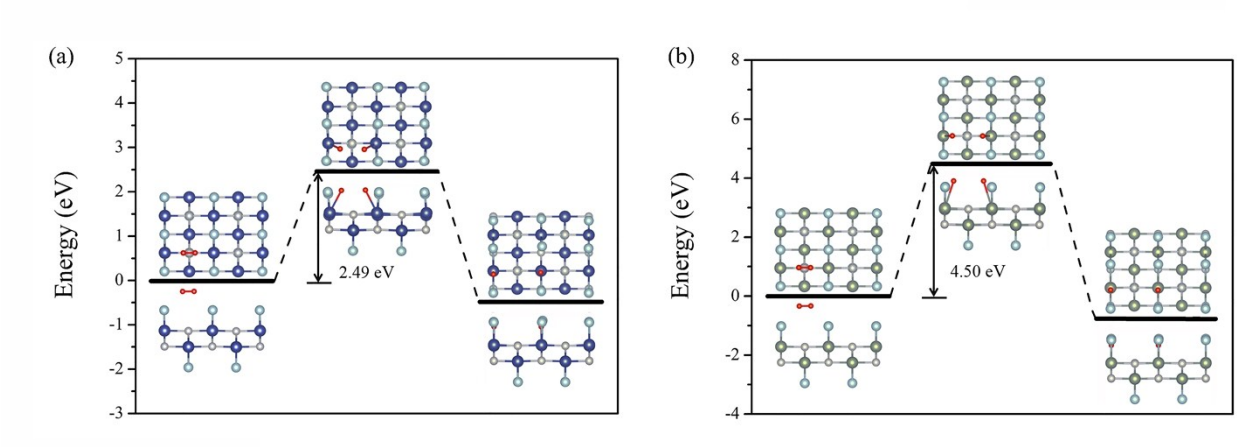

Fig. S6. The energy barrier for a physisorbed O_2 molecule to dissociate and chemisorb on the surface of (a) SL α-ZrPI and (b) SL α-HfPI.