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 $\alpha$-HfPI. (b) Variation of total energy of SL $\alpha$-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 $\alpha$-HfPI, (b) Possion’s ration of SL $\alpha$-ZrPI and (c) Possion’s ration of SL $\alpha$-HfPI as a function of the angle $\theta$ ($\theta = 0^\circ$ corresponds to the x axis).

Fig. S3. (a) The band structure and (b) projected density of states of SL $\alpha$-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 $\Gamma$ 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 \(\alpha\)-HfPI. (c) The partial charge density of VBM (left) at the \(\Gamma\) point and CBM (right) around the X point of SL \(\alpha\)-HfPI.

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

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

![Graphs showing phonon spectra of (a) SL \(\alpha\)-ZrPI and (b) SL \(\alpha\)-HfPI with the intermediate square lattice.](image)

**Fig. S5.** Phonon spectra of (a) SL \(\alpha\)-ZrPI and (b) SL \(\alpha\)-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 $\alpha$-ZrPI and (b) SL $\alpha$-HfPI.