Supplementary Materials for:

Carrier doping induced strong magnetoelastic coupling in 2D lattice

Yan Liang[1,*], Xingshuai Lv[2], Thomas Frauenheim[1,2,3,*]

[1]*Bremen Center for Computational Materials Science, University of Bremen, 28359 Bremen, Germany;*

[2]*Shenzhen JL Computational Science and Applied Research Institute, 518109 Shenzhen, P.R. China;*

[3]*Beijing Computational Science Research Center, 100193 Beijing, P.R. China.*

*Corresponding author:

yliang@uni-bremen.de (Y.L)

thomas.frauenheim@bccms.uni-bremen.de (T.F.)

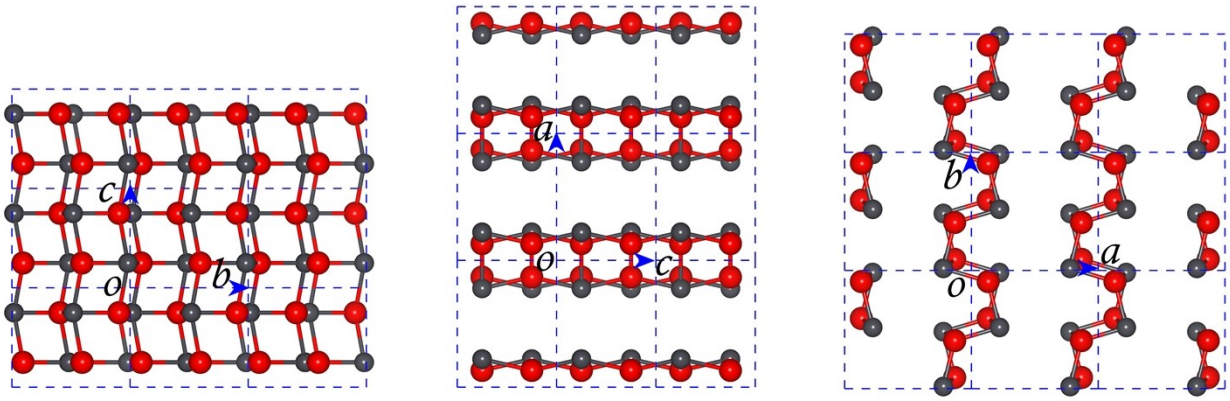

Figure S1. Top and side views of bulk β-PbO. The unit cell is distinguished by dashed lines.

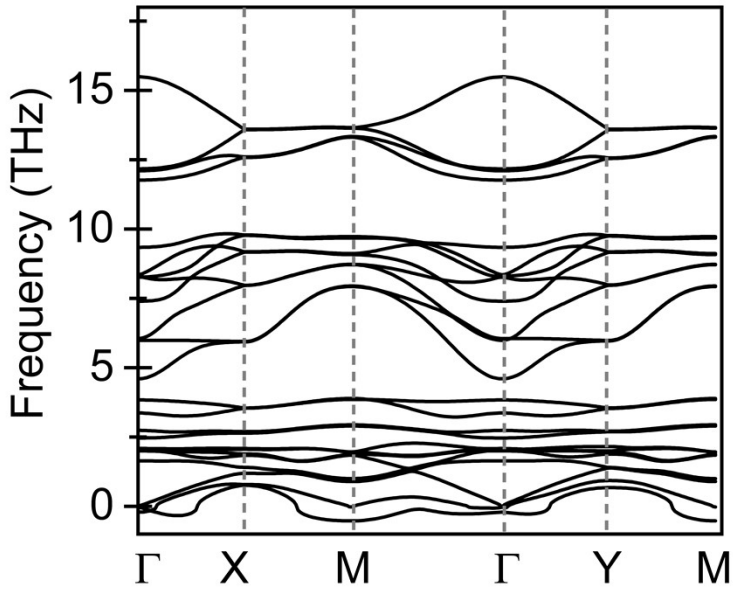

Figure S2. Phonon spectrum for 2D β-PbO at paraelastic state *P*.

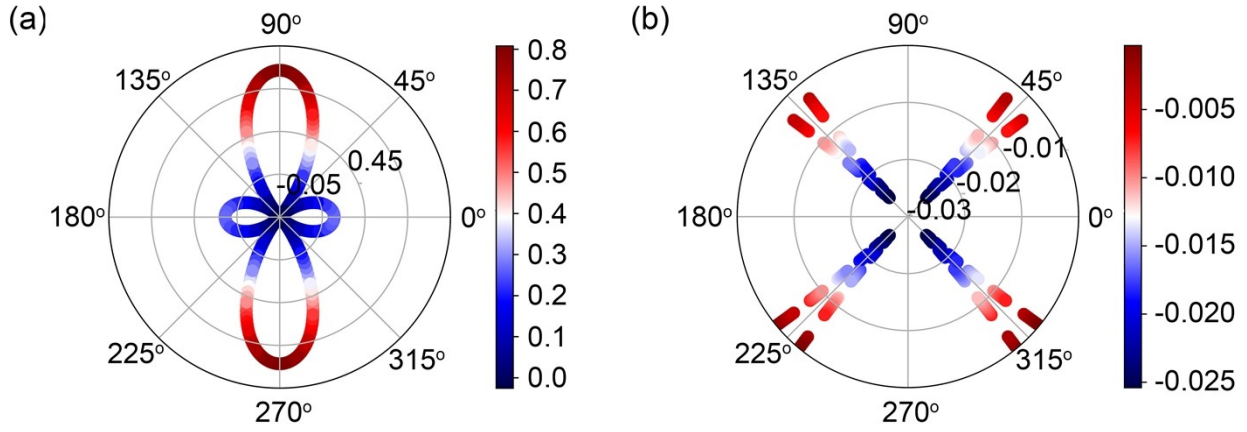

Figure S3. (a) Overall and (b) zoom in direction-dependent Possion's ratio of 2D β-PbO.

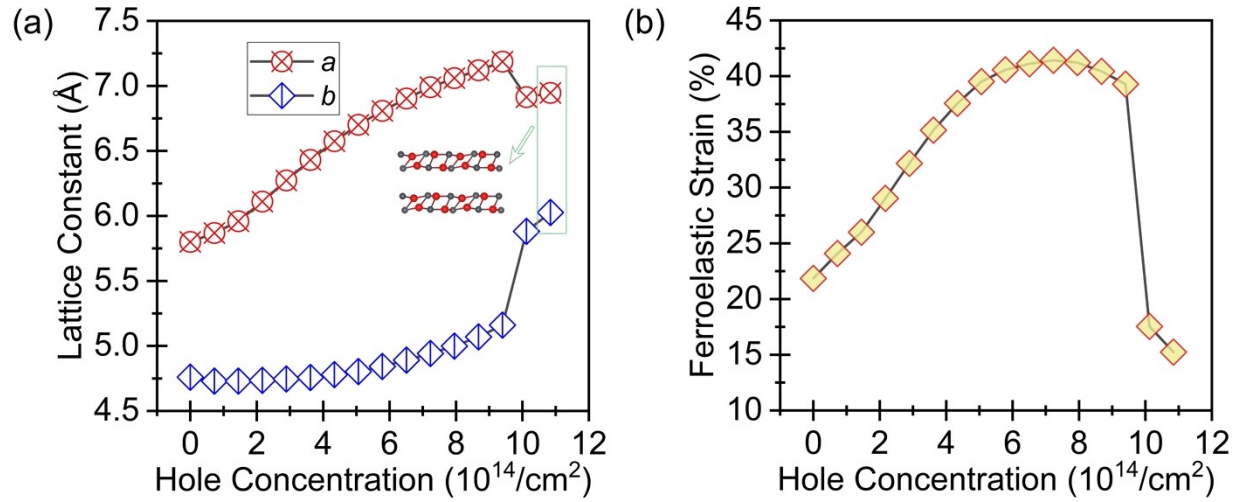

Figure S4. Doping concentration dependent (a) lattice constants and (b) ferroelastic strain for 2D β-PbO. The inset in (a) denotes the optimized one-dimensional like array for 2D β-PbO under doping density of $10.84 \times 10^{14}/cm^2$.

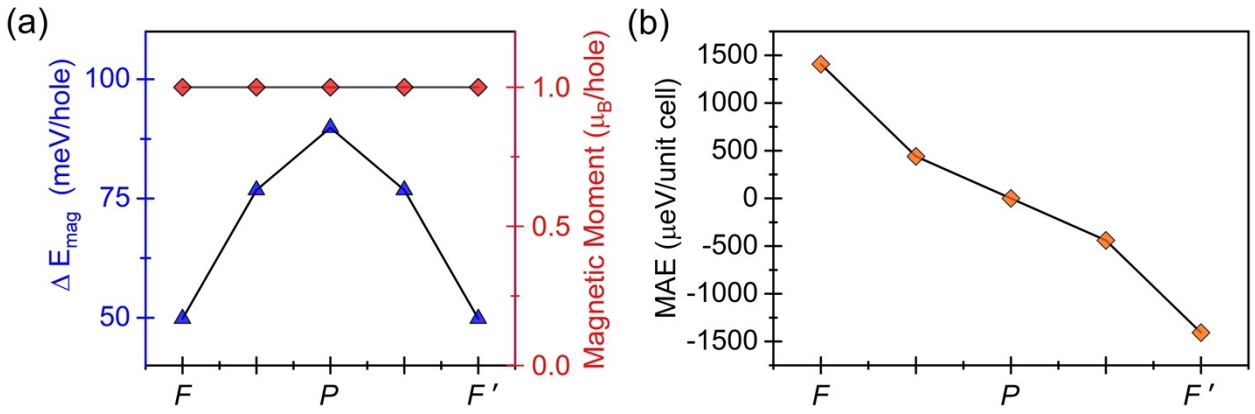

Figure S5. (a) The variation of the magnetic energy and magnetic moment (per carrier) and (b) MAE along with the ferroelastic transition at doping concentration of $7.23 \times 10^{14}/cm^2$.

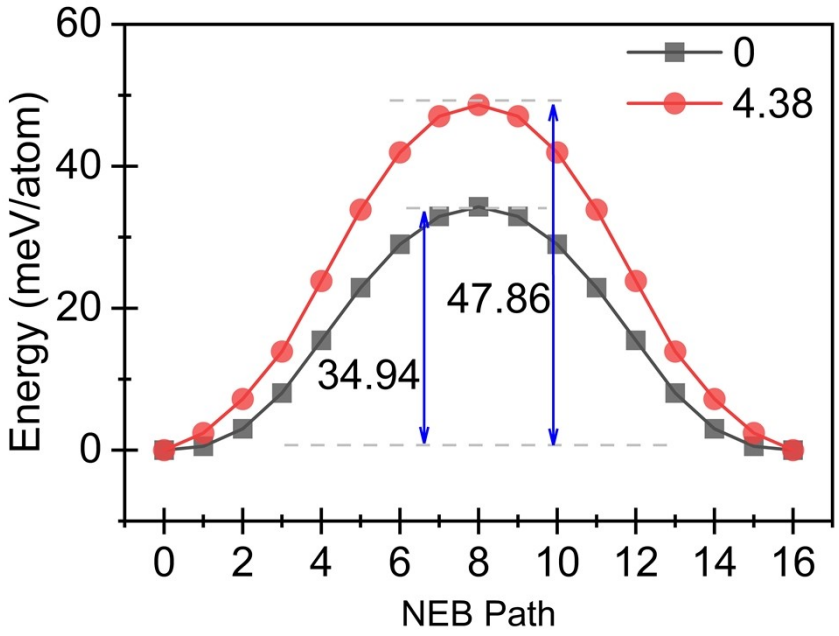

Figure S6. Energy barriers of ferroelastic switching for bilayer β-PbO under zero and $4.38 \times 10^{14}/cm^2$ hole doping concentration.

The lattice constants of bilayer β-PbO is calculated to be 5.76 Å and 4.75 Å. We check the possible doping-induced multiferroic phase in bilayer β-PbO by taking hole concentration of $4.38 \times 10^{14}/cm^2$ (1.2 hole per unit cell) as an example. Moderate ferroelastic switching barrier is displayed under doping, and it is found that ferromagnetic state is energetically more favorable than

non-magnetic state by 13 meV/hole. Additionally, the easy magnetization axis along in-plane [010] direction is more stable than [100] and [001] directions by 202 and 1104 μeV per unit cell, respectively. All these results support the strong magnetoelastic coupling in bilayer β-PbO under hole doping.