Supporting Information

Mechano-Ferroelectric Coupling: Stabilization Enhancement and Polarization Switching in Bent $AgBiP_2Se_6$ Monolayer

Jing Shang[1], Congxin Xia[2], Chun Tang [3], Chun Li[4], Yandong Ma[5], Yuantong Gu[1*], Liangzhi Kou[1*]

[1] School of Mechanical, Medical and Process Engineering, Queensland University of Technology, QLD, 4000, Australia

[2] College of Physics, Henan Normal University, Xinxiang, Henan 453007, China

[3] Faculty of Civil Engineering and Mechanics, Jiangsu University, No. 301 Xuefu Road, Zhenjiang, Jiangsu 212013, China

[4] School of Mechanics, Civil Engineering and Architecture, Northwestern Polytechnical University, Xi'an 710072, China

[5] School of Physics, State Key Laboratory of Crystal Materials, Shandong University, Shandanan Str. 27, Jinan 250100, China

Yuantong.gu@qut.edu.au; liangzhi.kou@qut.edu.au

1. FE phase transition from P↓ to P ↑ by bending in $AgBiP_2Se_6$ ribbons

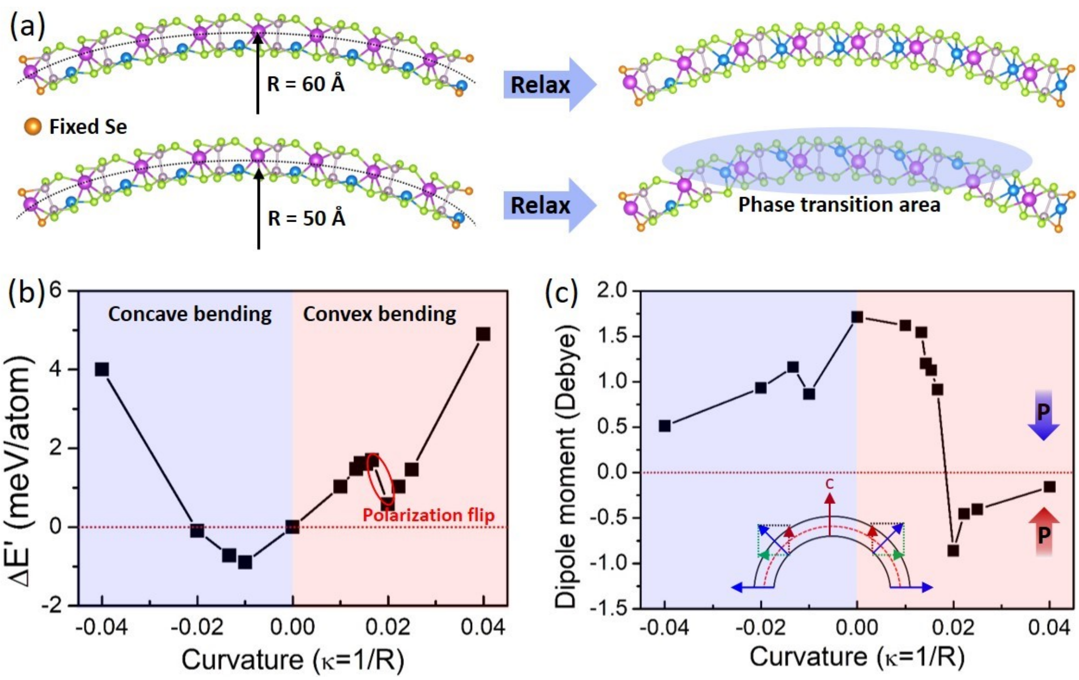

Figure S1. Bending in $AgBiP_2Se_6$ nanoribbons. (a): The relaxation from initial $AgBiP_2Se_6$ nanoribbon with Ag atoms locating at the bottom layer (left panel) to the relaxed ribbons with Ag atoms moving upwards (right panel). Accordingly, the ferroelectric polarization is reversed. The orange balls represent the fixed edge Se atoms. (b): The energy difference (ΔE') between nanoribbons with negative (left panel) and positive (right panel) curvatures and nonperiodic flat $AgBiP_2Se_6$ nanoribbon. The insets are the bending directions for P ↓ $AgBiP_2Se_6$ nanoribbons including up-bending (left) and down-bending (right). (c): The dipole moments (Debye) of the bent nanoribbons with various curvatures.

2. FE phase transition from P↓ to P ↑ by bending in In_2Se_3 monolayer

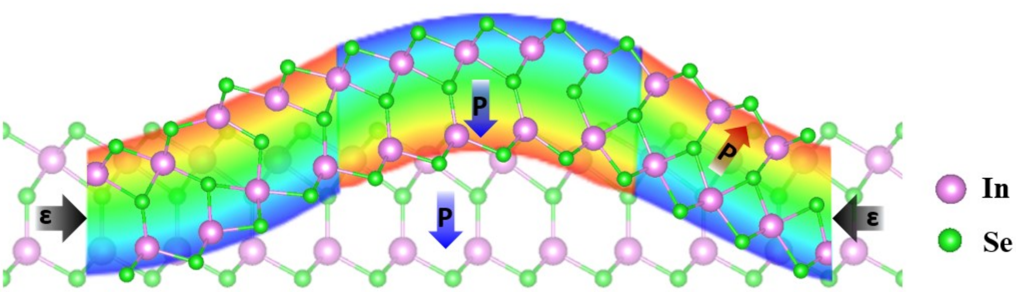

Fig. S2. Structures with and without bending deformation in In_2Se_3 monolayer. The bending deformation in P ↓ In_2Se_3 monolayer is resulted by the in-plane compressive strain of $\varepsilon = 0.08$, as labelled by black arrows. The blue and red arrows indicate the FE polarizations in In_2Se_3 monolayer. With bending load, the FE polarization in compressive area flips form P ↓ to P ↑.

3. The size effect of ferroelectric bubble in $AgBiP_2Se_6$ monolayers

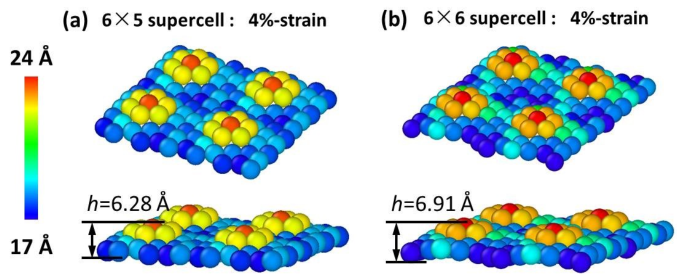

Fig. S3. Ferroelectric bubble with hights (*h*) in biaxially rippled $AgBiP_2Se_6$ monolayers. (a): 6×5 supercell with 4% biaxial strain; (b) :6×6 supercell with 4% biaxial strain.