Supplementary Information
Two-dimensional Arsenene Polymorph Beyond the Auxetic Foam: High Mechanical Sensitivity and Large, Negative NPR

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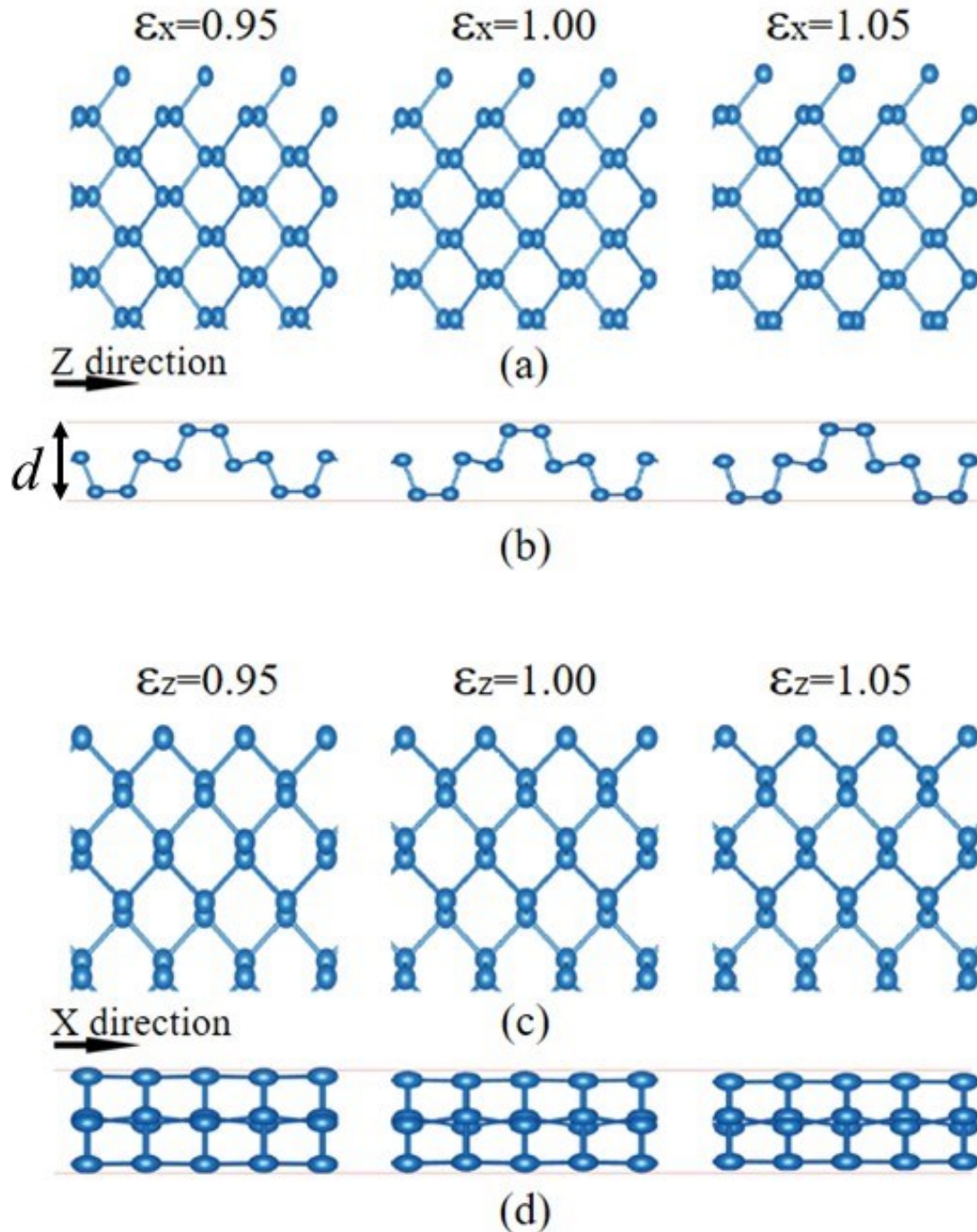
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Figure S1 (a) Top views of the configuration of single-layer δ-As under uniaxial deformation at strain states of ε=0.95, 1.00, 1.05 in the X direction. (b) Side views of the configuration of single-layer δ-As under uniaxial deformation at strain states of ε=0.95, 1.00, 1.05 in the X direction. (c) Top views of the configuration of single-layer δ-As under uniaxial deformation at strain states of ε=0.95, 1.00, 1.05 in the Z direction. (d) Side views of the configuration of single-layer δ-As under uniaxial deformation at strain states of ε=0.95, 1.00, 1.05 in the Z direction.

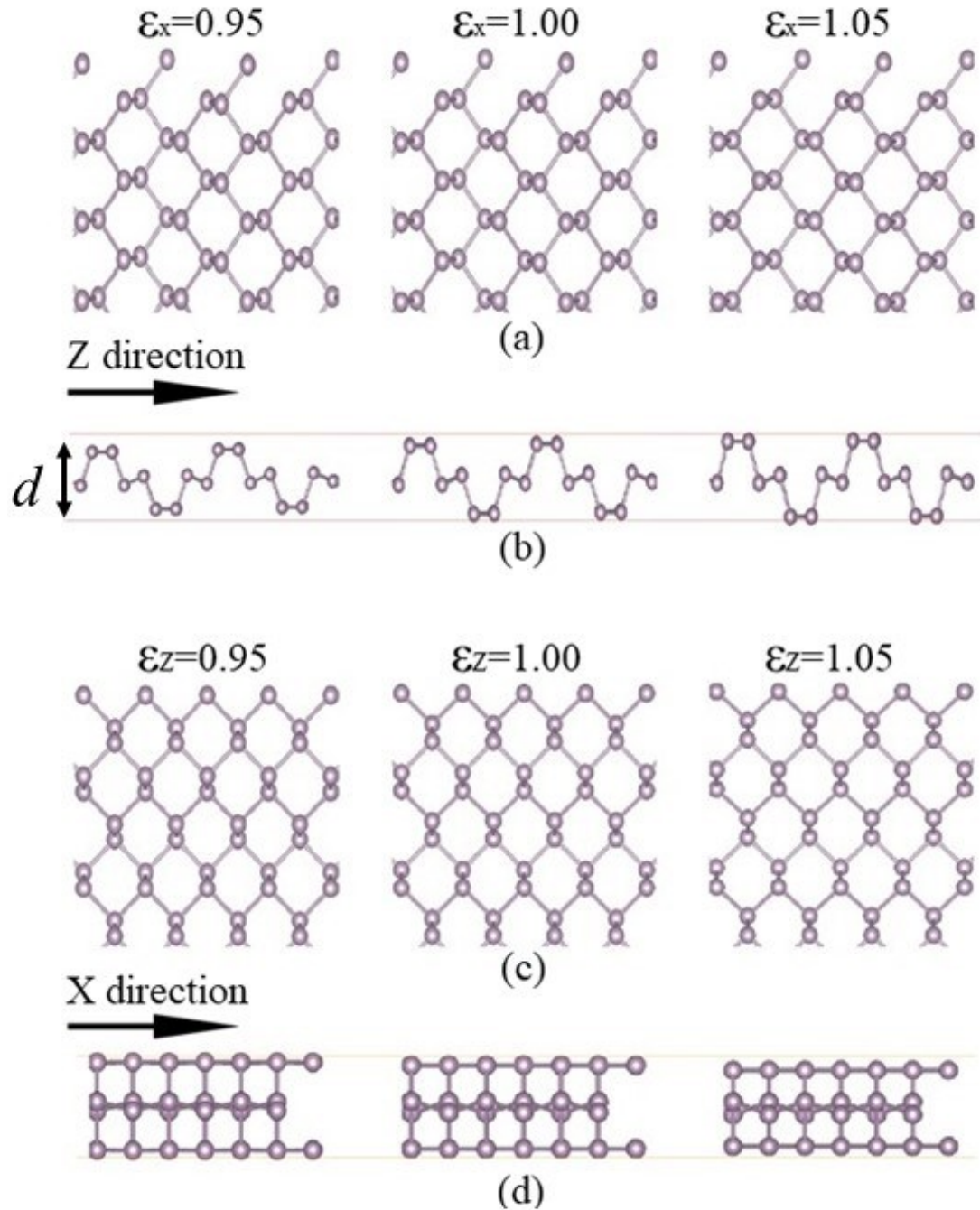**Figure S2** (a) Top views of the configuration of single-layer γ-P under the X-direction deformation at strain states of ε=0.95, 1.00, 1.05. (b) Side views of the configuration of single-layer γ-P under the X-direction deformation at strain states of ε=0.95, 1.00, 1.05. (c) Top views of the configuration of single-layer γ-P under the Z-direction deformation at strain states of ε=0.95, 1.00, 1.05. (d) Side views of the configuration of single-layer γ-P under the Z-direction deformation at strain states of ε=0.95, 1.00, 1.05.
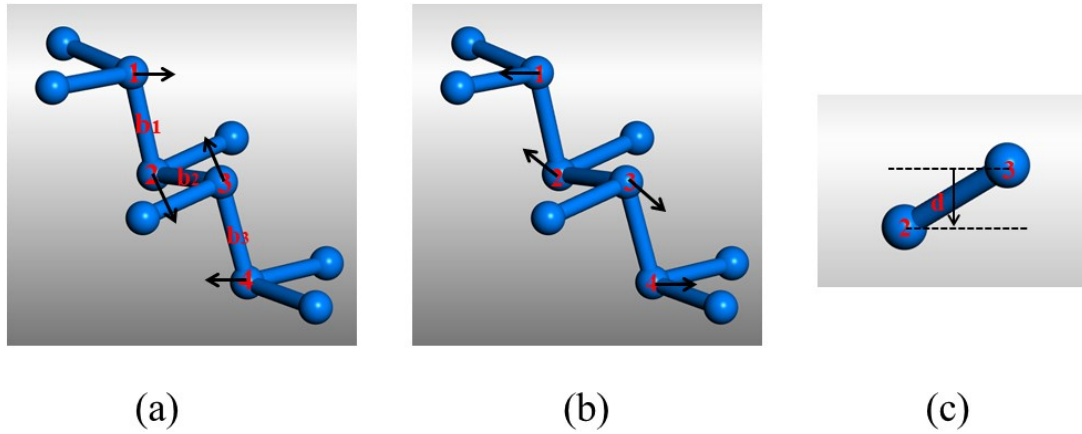
Figure S3 Evolution of local structure in single-layer δ-As during uniaxial tension in the X direction. (a) Single-layer δ-As is stretched in the X direction, that is, atoms are moved in the direction of the attached arrows (black online). (b) Single-layer δ-As is contracts in the X direction, that is, atoms are moved in the direction of the attached arrows (black online). (c) Vertical distance d between atoms 2 and 3 under the X-direction uniaxial tension and compression strain.
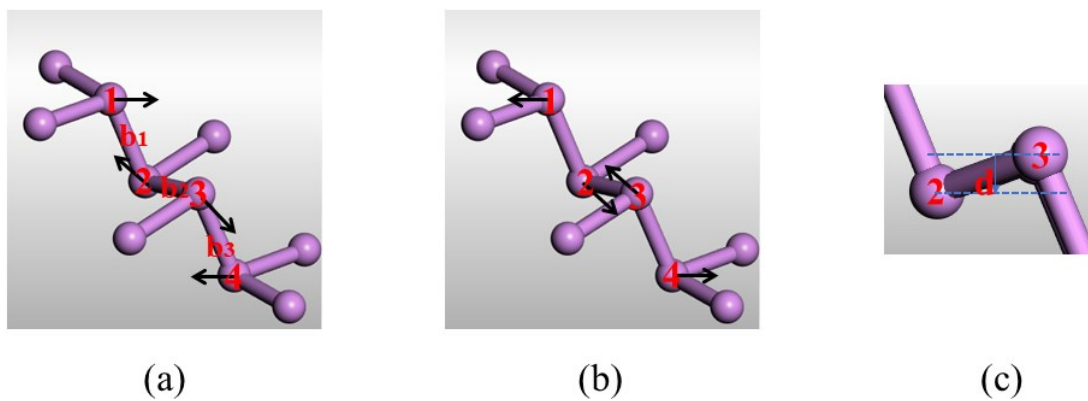
Figure S4 Evolution of local structure in single-layer γ-P during uniaxial tension in the X direction. (a) Single-layer γ-P is stretched in the X direction, that is, atoms are moved in the direction of the attached arrows (black online). (b) γ-P is contracts in the X direction, that is, atoms are moved in the direction of the attached arrows (black online). (c) Vertical distance *d* between atoms 2 and 3 under the X-direction uniaxial tension and compression strain.