Supporting Information

Mechanically-Controllable Strong 2D Ferroelectricity and Optical Properties of Semiconducting BiN Monolayer

Peng Chen, Xue-Jing Zhang, and Bang-Gui Liu*

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

*Email: bgliu@iphy.ac.cn

1. Total-energy comparison of the BiN monolayer with other similar 2D structures

	BiN	CuI-like [1]	SiP-like [2]	InSe-like [3]	GeTe-like [4]	GaSe-like [5]	BN-like [6]
Energy (eV/f.u.)	-11.78267	-11.56397	-11.44983	-11.05758	-11.04598	-11.02103	-10.44433

[1] Synthesis of ultrathin two-dimensional nanosheets and van der Waals heterostructures from non-layered γ-CuI, npj 2D Materials and Applications **2**, 16 (2018)

[2] Two-dimensional SiP: an unexplored direct bandgap semiconductor, 2D Mater. **4**, 015030 (2017)

[3] InSe: a two-dimensional material with strong interlayer coupling, Nanoscale **10**, 7991 (2018)

[4] Sonication-assisted liquid-phase exfoliated α-GeTe: a two-dimensional material with high Fe3+ sensitivity, Nanoscale **10**, 15989 (2018)

[5] Multifunctional 2D- Materials: Gallium Selenide, Materials Today: Proceedings **4**, 5471 (2017)

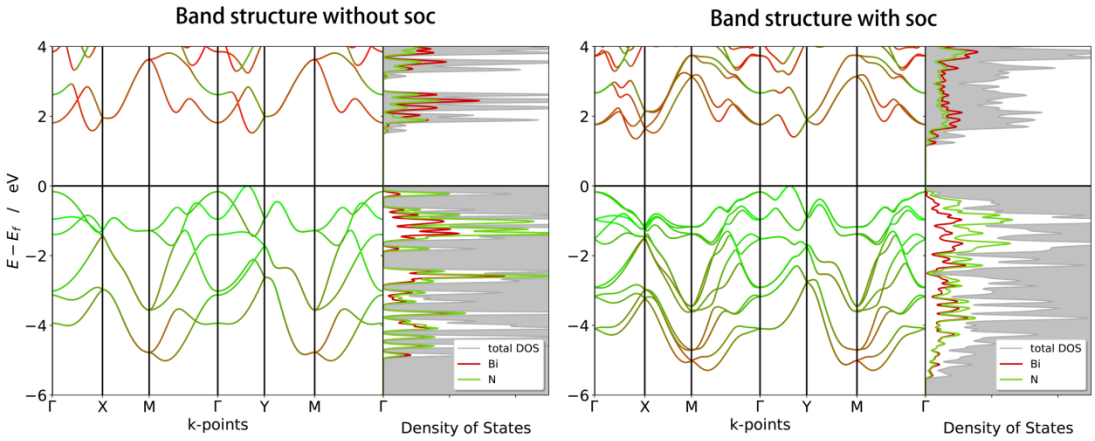
[6] B/C/N Materials Based on the Graphite Network, Adv Mater **8**, 9 (1997)

2. **Structural parameters under uniaxial stress.**

Strain	-5.0%	-2.0%	0.0%	2.0%	-2.0%	0.0%	2.0%	5.0%
Lattice constant	a=3.2960 b=3.6767 c=15.000 γ =90	a=3.4000 b=3.6478 c=15.000 γ =90	a=3.4694 b=3.6287 c=15.000 γ =90	a=3.5388 b=3.6070 c=15.000 γ =90	a=3.5380 b=3.4749 c=15.000 γ =90	a=3.6287 b=3.4694 c=15.000 γ =90	a=3.7194 b=3.4619 c=15.000 γ =90	a=3.8101 b=3.4556 c=15.000 γ =90
Wyckoff position	Bi: 0.0000 0.5527 0.4617 N: 0.0000 0.4473 0.6055	Bi 0.0000 0.5551 0.4626 N: 0.0000 0.4449 0.6059	Bi: 0.0000 0.5567 0.4631 N: 0.0000 0.4433 0.6062	Bi: 0.0000 0.5578 0.4637 N: 0.0000 0.4422 0.6064	Bi: 0.0489 0.5000 0.6376 N: 0.9511 0.5000 0.4938	Bi: 0.0567 0.5000 0.6369 N: 0.9433 0.5000 0.4938	Bi: 0.0630 0.5000 0.6361 N: 0.9370 0.5000 0.4938	Bi: 0.0689 0.5000 0.6354 N: 0.9311 0.5000 0.4939

Eight structures are given in the table. All of them are from the lowest energy phases from fig3 (a). More precisely, the first 4 structures belong to the ferroelectric [010] phase under strain, and the remaining 4 structures belong to the ferroelectric [100] phase. The 3rd and 6th columns describe the minima of the [010] and [100] phases, respectively. The 4th and 5th columns describe the two phases the crossing at the transition point in fig3 (a).

3. Effect of the spin-orbits coupling on the band structures



The band structures and density of states (DOS) of the BiN monolayer without and with (the left and the right) the spin-orbit coupling (soc).