Supporting Information

A Novel SiO Monolayer with Negative Poisson's Ratio and Dirac Semimetal

Hui Du[1], Guoling Li[2], Jiao Chen [3], Zhenlong Lv [1], Yuanzheng Chen[3*], Shijie Liu[1, 4*]

[1] Henan Key Laboratory of Photoelectric Energy Storage Materials and Applications, School of Physics and Engineering, Henan University of Science and Technology, Luoyang, 471023, China

[2] Chemistry and Chemical Engineering Guangdong Laboratory, Shantou 515031, China

[3] School of Physical Science and Technology, Key Laboratory of Advanced Technologies of Materials, Ministry of Education of China, Southwest Jiaotong University, Chengdu 610031, China

[4] State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, China.

* Corresponding authors

E-mail: liusj0228@163.com, cyz@calypso.org.cn

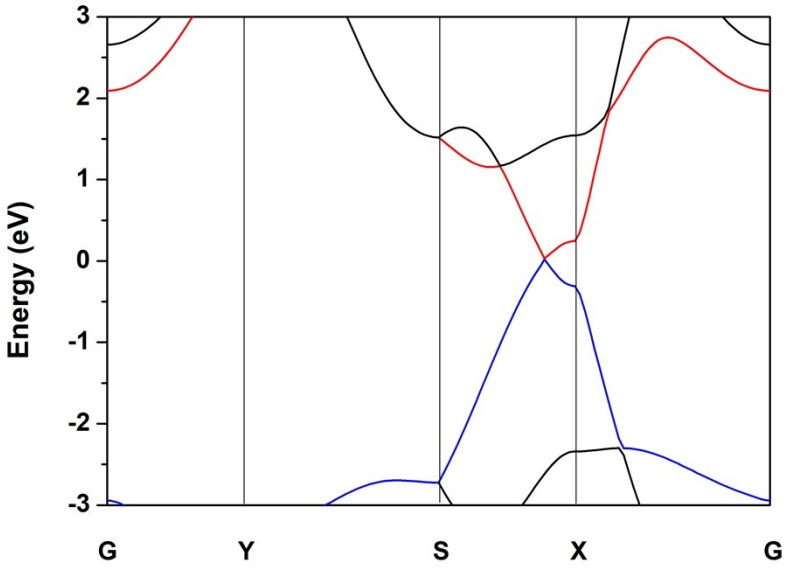

Figure S1. The band structure of Pmna by HSE method.

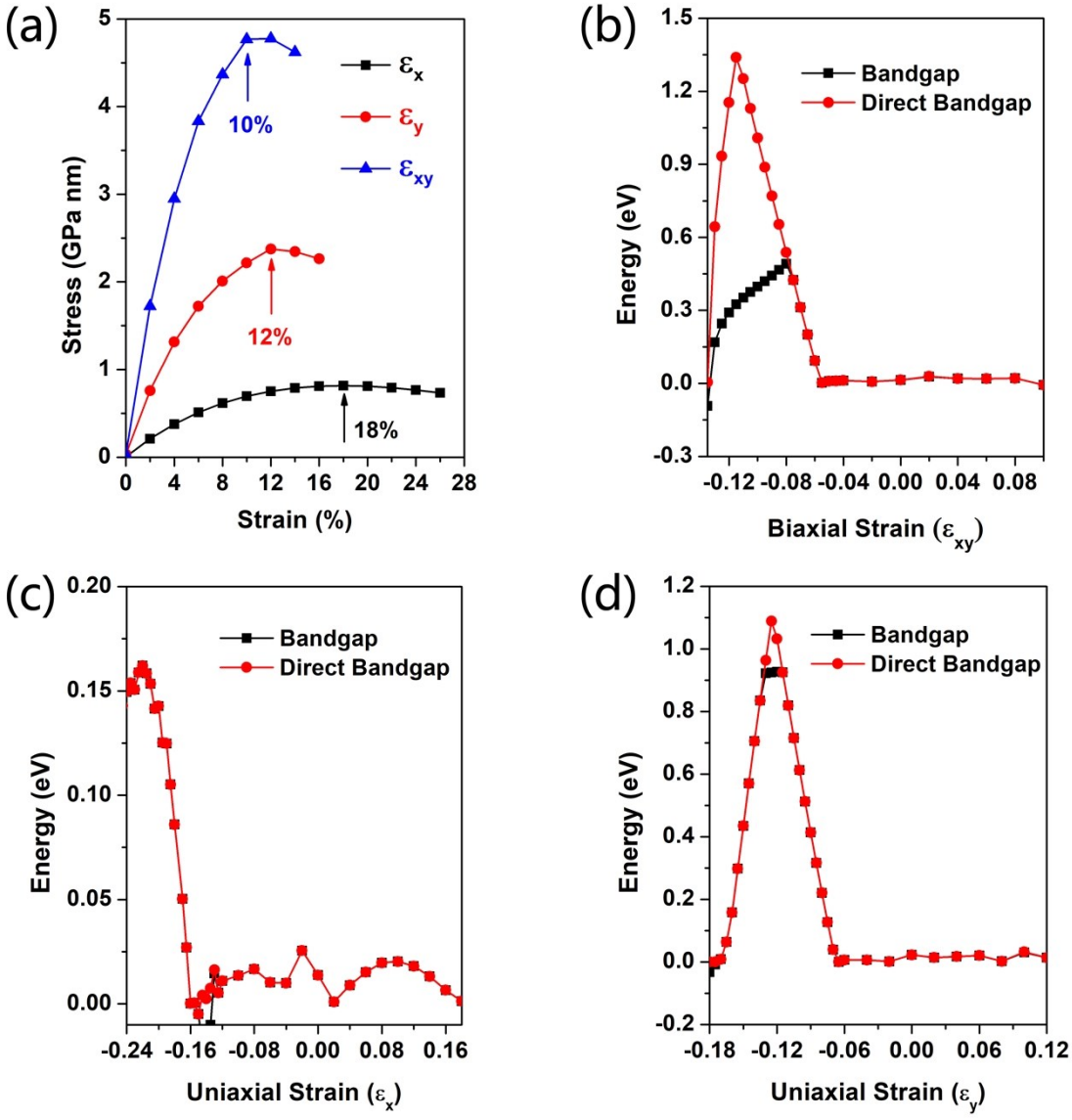

Figure S2. The calculated stress (a) versus the applied strain and bandgap along xy (b), x (c) and y (d) of Pmna structure.

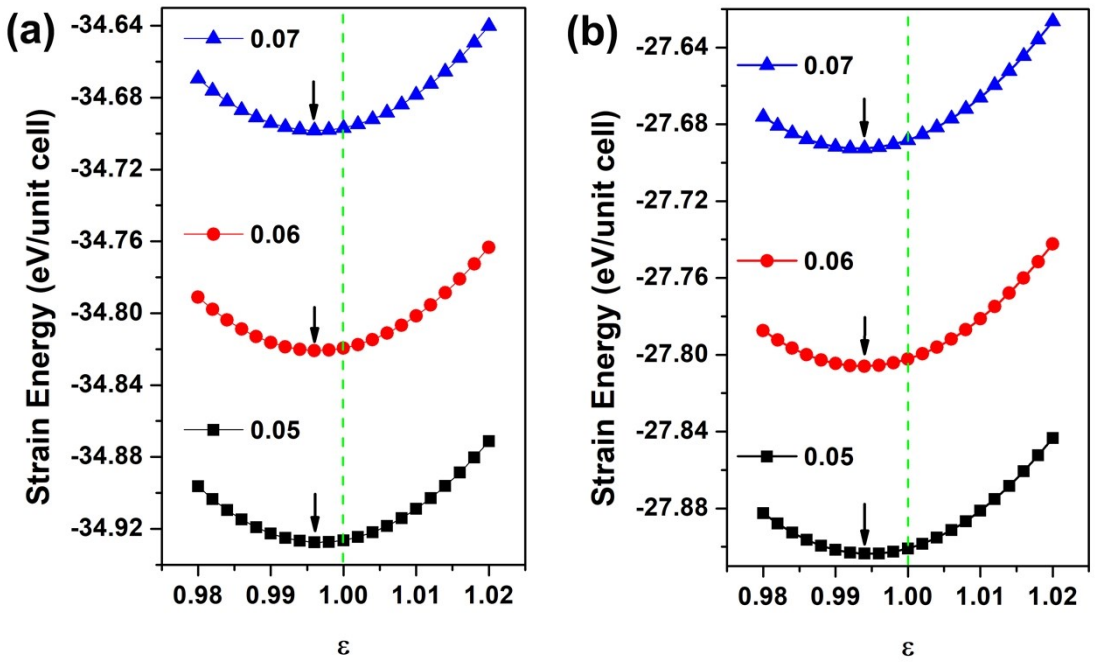

Figure S3. Total energy with respecting to lattice response of the other direction when the BN AB stack (a) and SiC AB stack (b) lattice is under 5%, 6% and 7% tensile strain along y directions, respectively. The arrows indicate the equilibrium magnitude of ε.

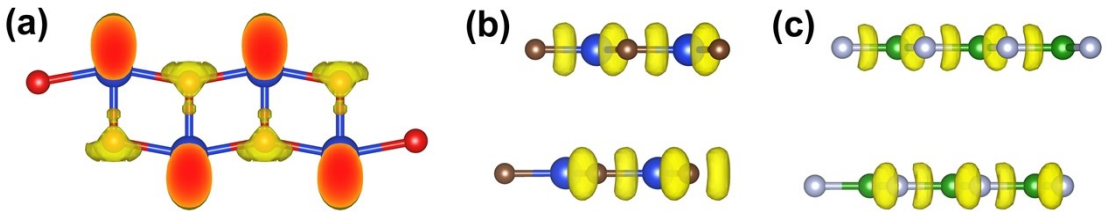

Figure S4. The calculated ELF of 2D SiO (a) and SiC AB stack (b) and BN AB stack (c), respectively.