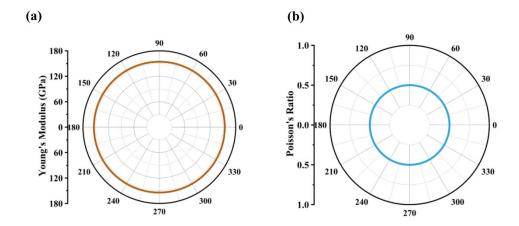
Supplementary Information (SI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2025

## $\label{eq:Supplementary Information} Supplementary\ Information$ Planar Fe\_2B Monolayer with Room Temperature Antiferromagnetism

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 $\textbf{Fig. S1} \ (a) \ Young's \ modulus \ and \ (b) \ Poisson's \ ratio \ of the \ Fe_2B \ monolayer.$ 

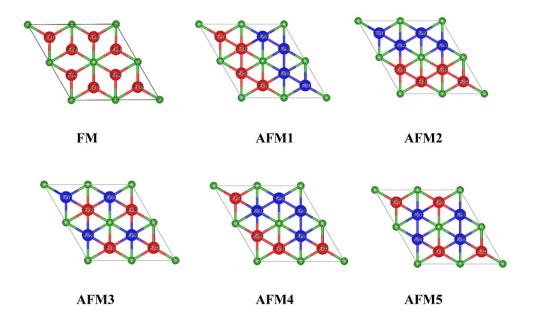


Fig. S2 Six different magnetic configurations of the  $Fe_2B$  monolayer, the red and blue balls represent spin-up and spin-down Fe atoms, respectively.

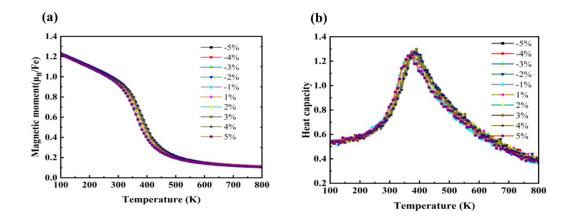


Fig. S3 (a) The temperature-depended  $M_Z$  and (b)  $C_V$  the Fe<sub>2</sub>B monolayer under biaxial strain.

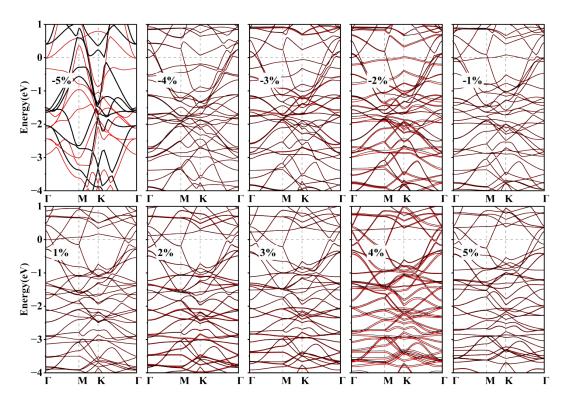


Fig. S4 Spin-polarized band structure of the Fe<sub>2</sub>B monolayer under biaxial strain.

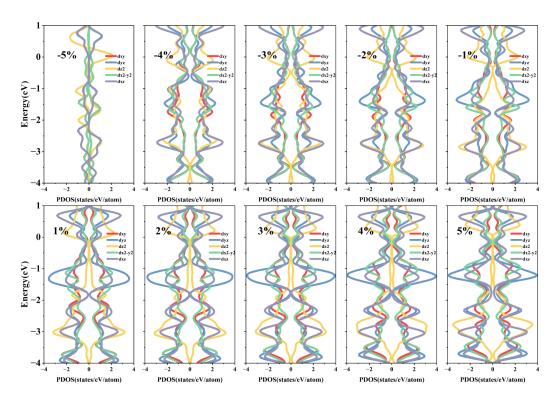


Fig. S5 Partial density of states (PDOS) of Fe atoms in the Fe<sub>2</sub>B monolayer under biaxial strain.