Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY MATERIAL

Compression-Induced Crimping of Boron Nanotubes from Borophenes : A DFT Study

Xueqin Qin[a], Jia Liu[a], Yuewen Mu[*a], and Si-Dian Li[*a]

[a] *Key Laboratory of Materials for Energy Conversion and Storage of Shanxi Province, Institute of Molecular Science, Shanxi University, Taiyuan 030006, China.*
E-mail: ywmu@sxu.edu.cn ; lisidian@sxu.edu.cn .

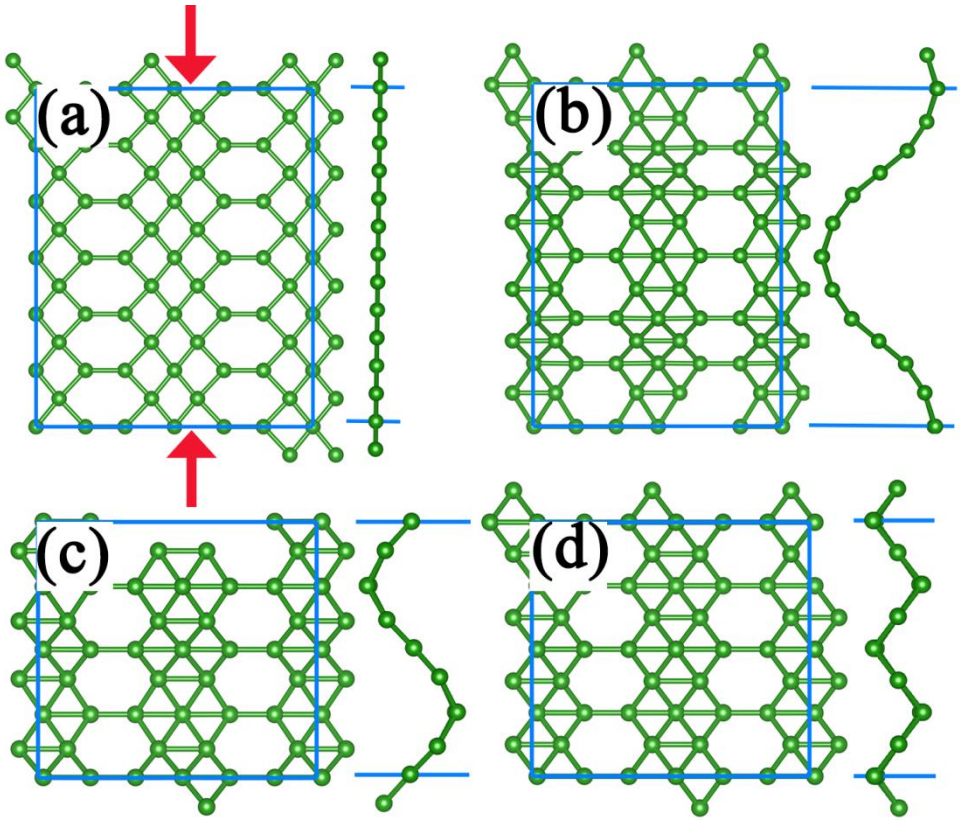

Figure S1. Top and side views of compressed β_{12} borophene under $\varepsilon_b = 20\%$ for (a) plane-*b*, (b) ripple-6*b*, (c) ripple-4*b* and (d) ripple-2*b* modes.

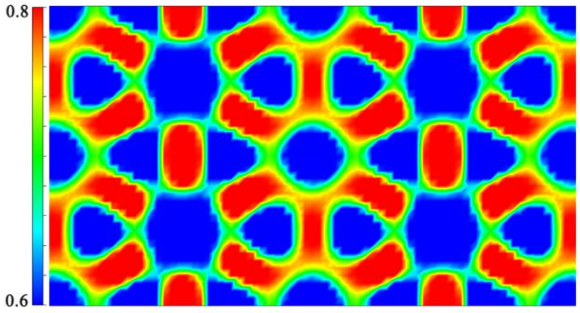

Figure S2. Electron localization function (ELF) plot in the basal plane of the β_{12} borophene. The isovalue is 0.6~0.8.

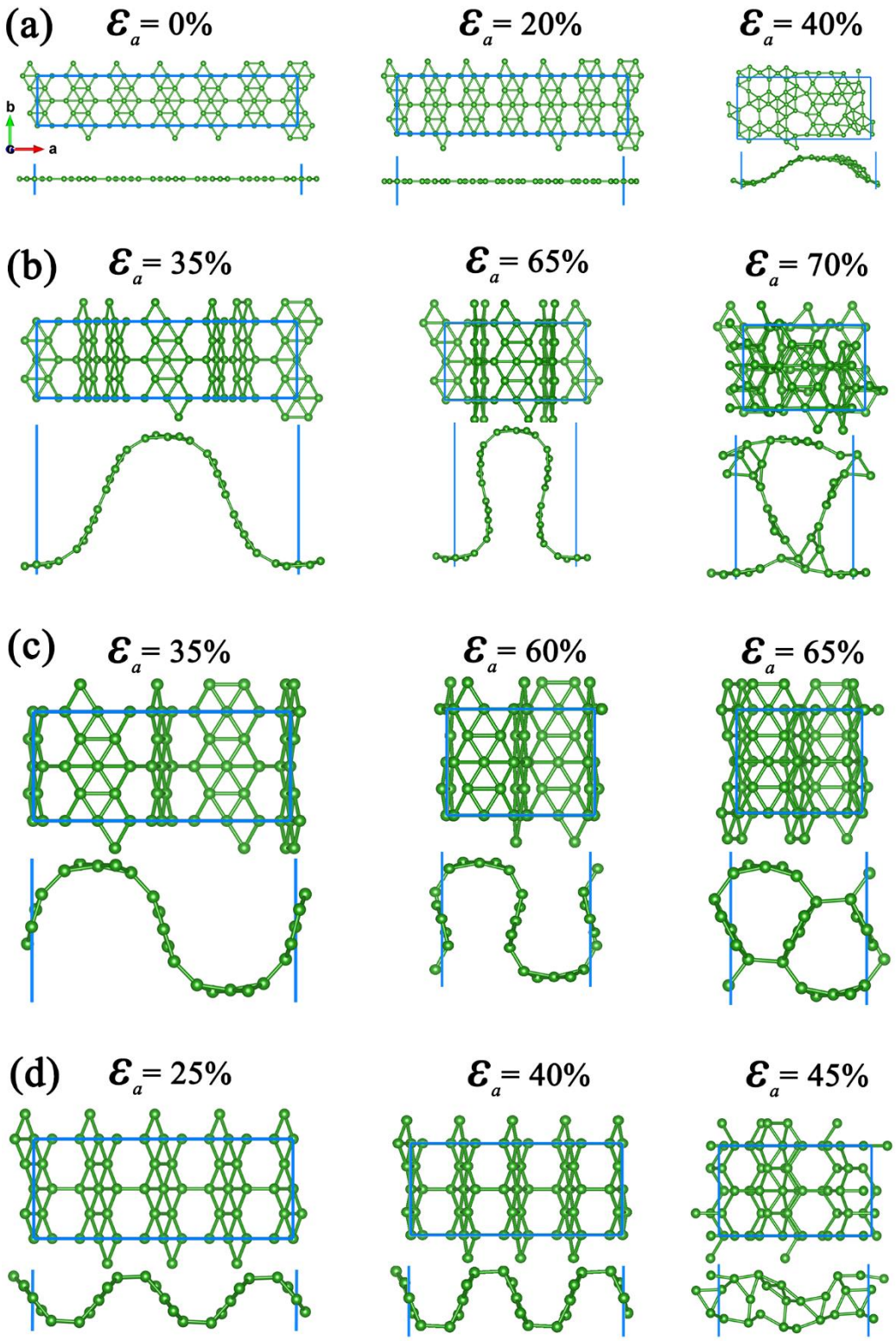

Figure S3. Top and side views of the geometries of β_{12} borophene under different compressions ε_a for (a) plane-*a*, (b) ripple-6*a*, (c) ripple-4*a* and (d) ripple-2*a* modes.

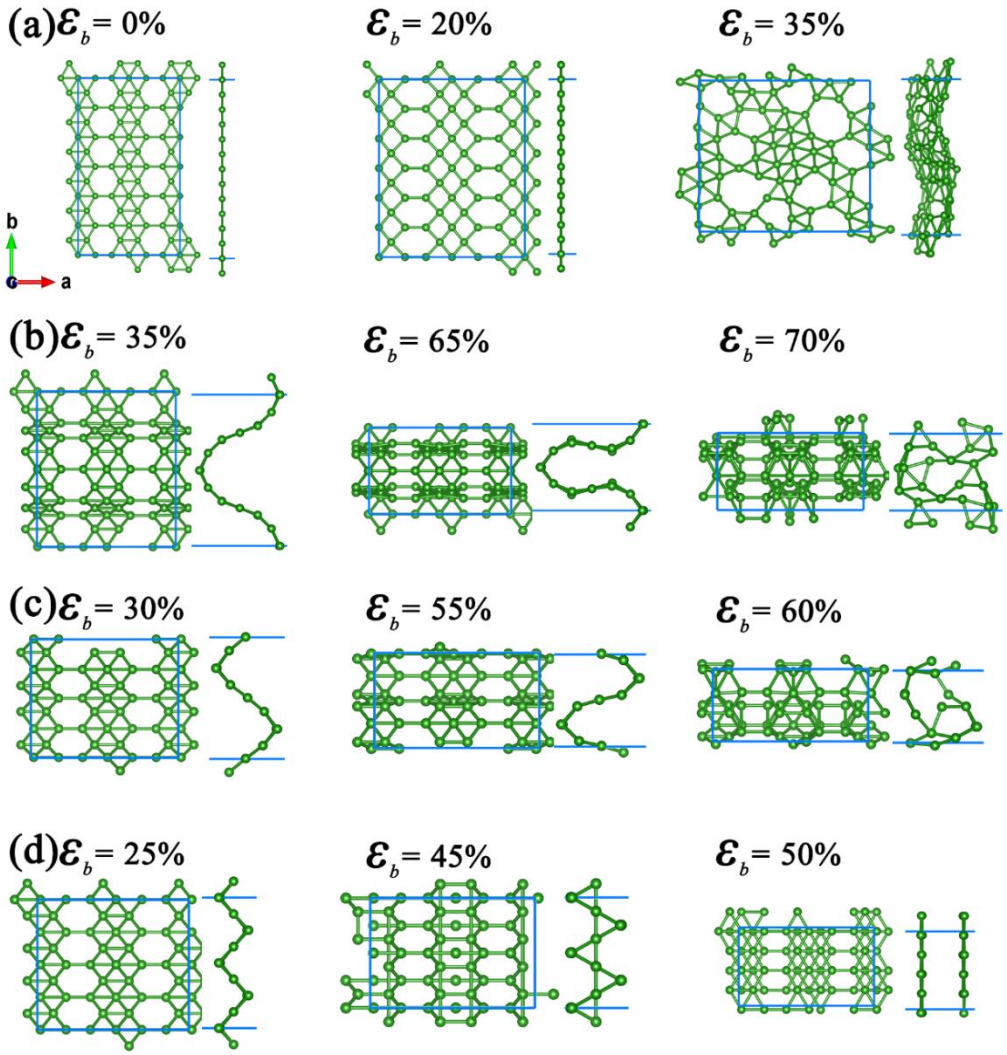

Figure S4. Top and side views of the geometries of β_{12} borophene under different compressions ε_b for (a) plane-*b*, (b) ripple-6*b*, (c) ripple-4*b* and (d) ripple-2*b* modes.

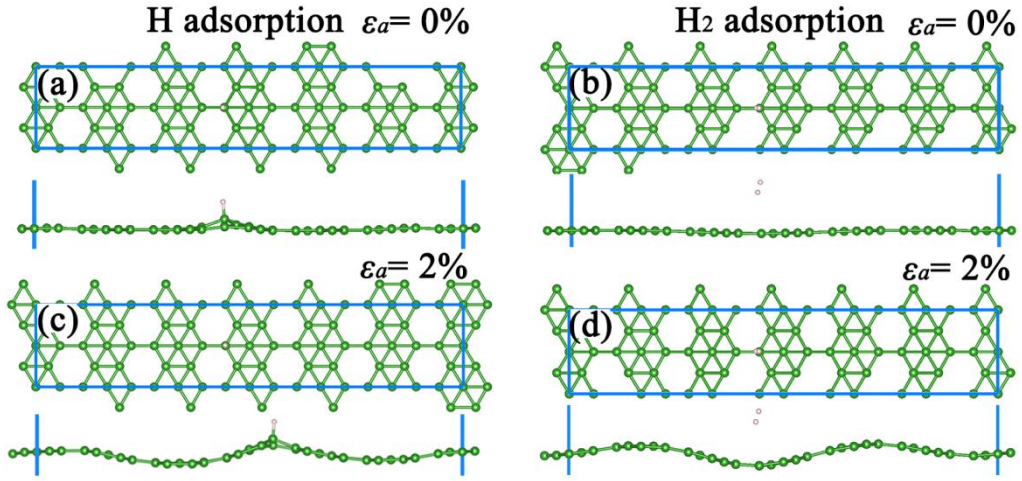

Figure S5. Top and side views of optimized plane β_{12} borophene with an H adatom under the compressions of (a) $\varepsilon_a = 0\%$ and (c) $\varepsilon_a = 2\%$, or with an H_2 molecule under the compressions of (b) $\varepsilon_a = 0\%$ and (d) $\varepsilon_a = 2\%$.

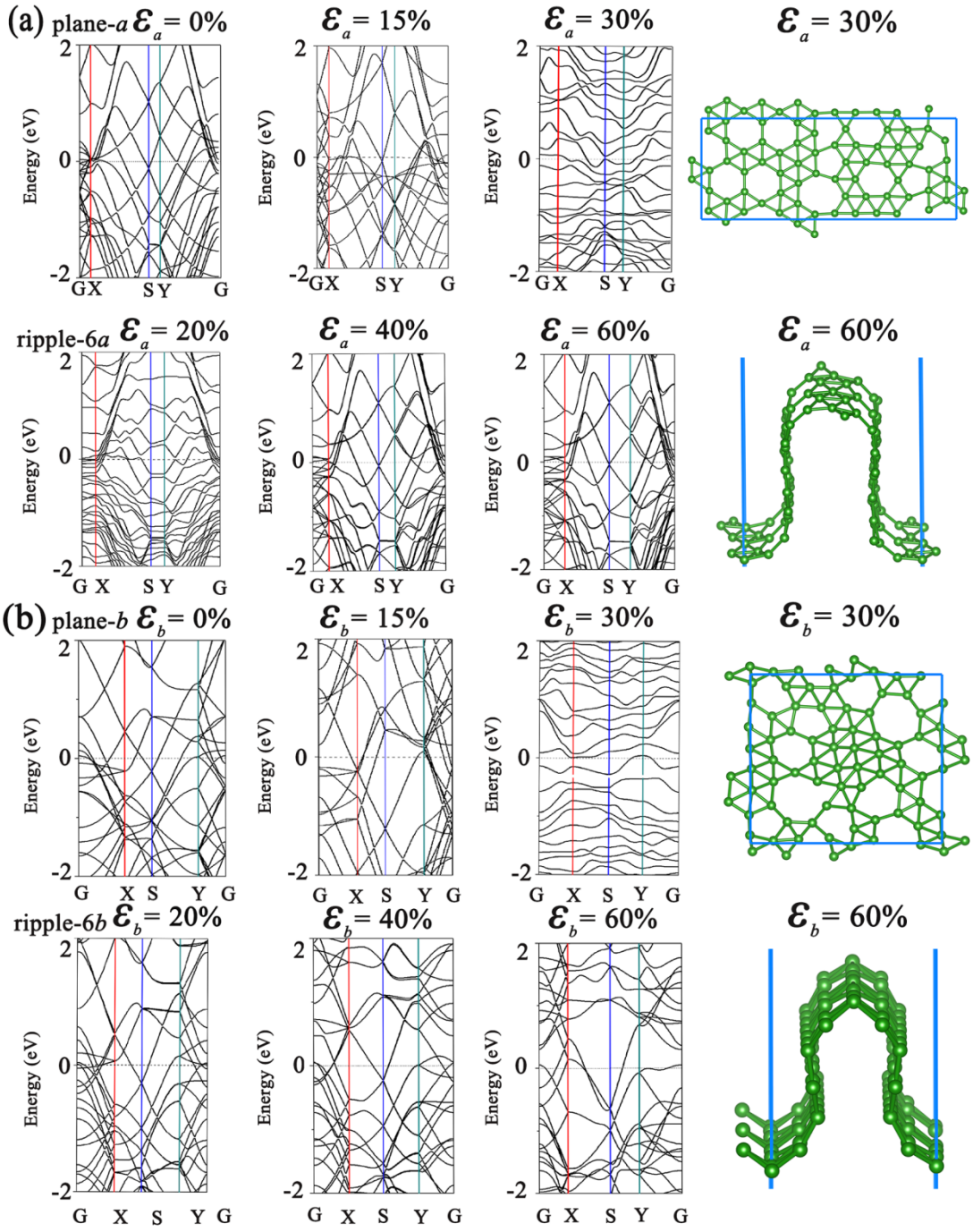

Figure S6. Band structures of β_{12} borophene under compressive strains in the (a) *a* and (b) *b* directions.

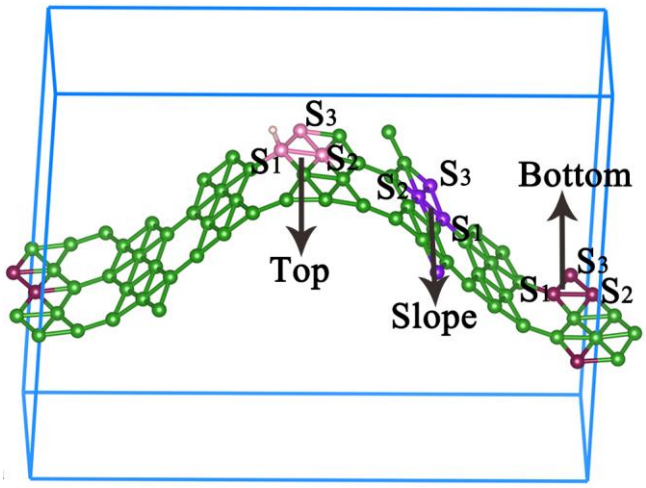

Figure S7. Adsorption sites of an H adatom on different parts of the compressed ripple-6*a* borophene ($\varepsilon_a = 20\%$).

Table S1. Adsorption free energy (ΔG_H) of the hydrogen atom on different parts of the compressed ripple-6*a* borophene ($\varepsilon_a = 20\%$).

Part	ΔG_H-S_1 (eV)	ΔG_H-S_2 (eV)	ΔG_H-S_3 (eV)
Top	-0.02614263	1.12836773	0.0593748
Slop	0.09355775	0.98886098	0.15969585
Bottom	0.24177152	1.03724612	0.34494609

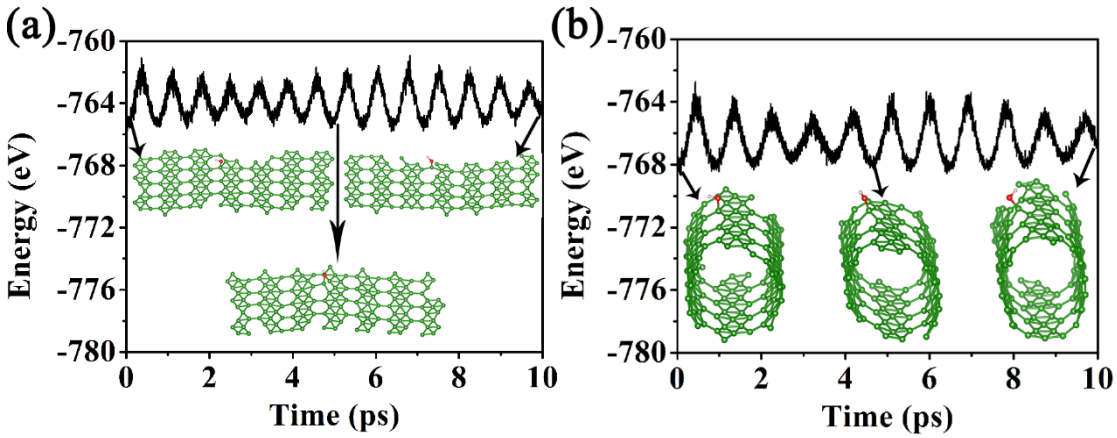

Figure S8. Energy evolution and snapshots of (a) plane β_{12} borophene and (b) boron nanotube (6,0) with OH during the AIMD simulation at 300 K.