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RESEARCH ARTICLE

Ab initio study of anisotropic mechanical and electronic properties of strained carbon-nitride nanosheet with interlayer bonding

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SUPPLEMENTARY MATERIAL

Table 1 The calculated structure parameters of CN nanosheet in LB (low-buckled) geometry without interlayer bonding and planar (PL) geometry. The values of angle between intralayer bond C-N-C (α), C-N bond length (d_{CN}), lattice constant (a), and cohesive energy (E_{coh}) are given.

Structure	α (°)	d_{CN} (Å)	a (Å)	E_{coh} (eV/atom)
LB geometry without interlayer bonding	119.1	1.390	2.396	7.994
Planar geometry	120.0	1.385	2.399	7.992

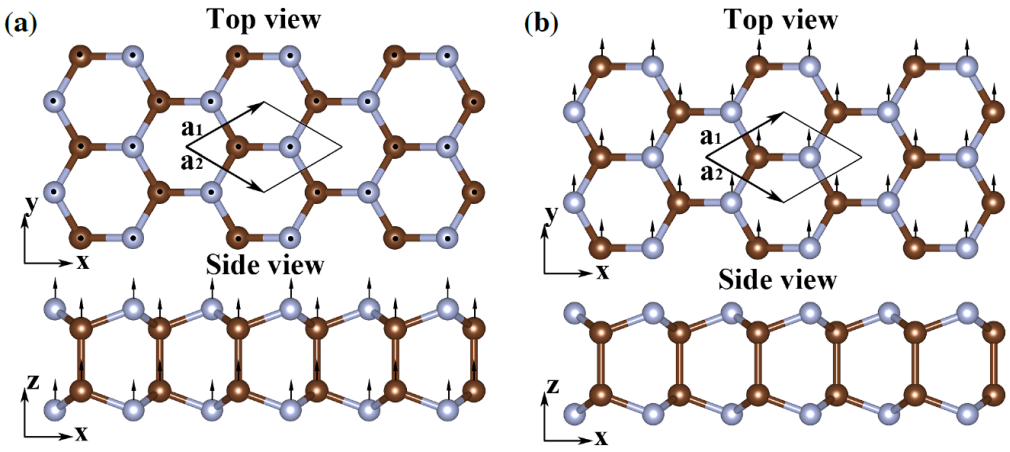

Fig. 1 The illustration of unstable eigenvector corresponding to **(a)** out-of-plane transverse phonon branch ZA at $\varepsilon_{xx} = 0.13$ and **(b)** in-plane transverse phonon branch TA at $\varepsilon_{yy} = 0.18$.

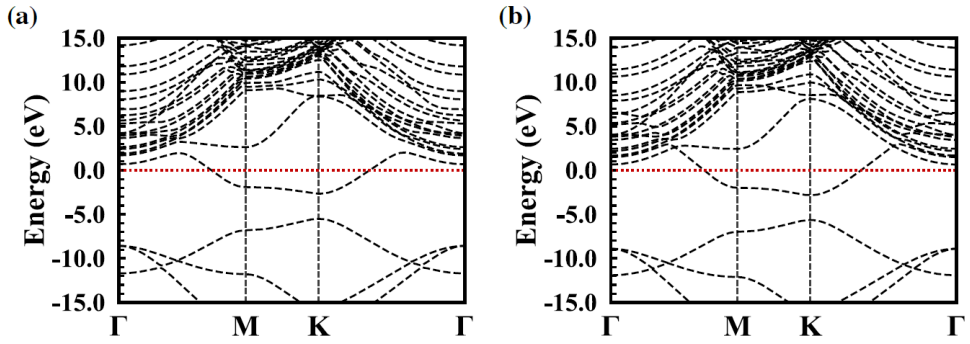

Fig. 2 Calculated electronic band structures of CN nanosheet in **(a)** LB geometry without interlayer bonding and **(b)** planar (PL) geometry are presented. The Fermi energy is set to be zero.