

## Electronic Supplementary Information

### Three metallic BN polymorphs: 1D multi-threaded conduction in 3D network

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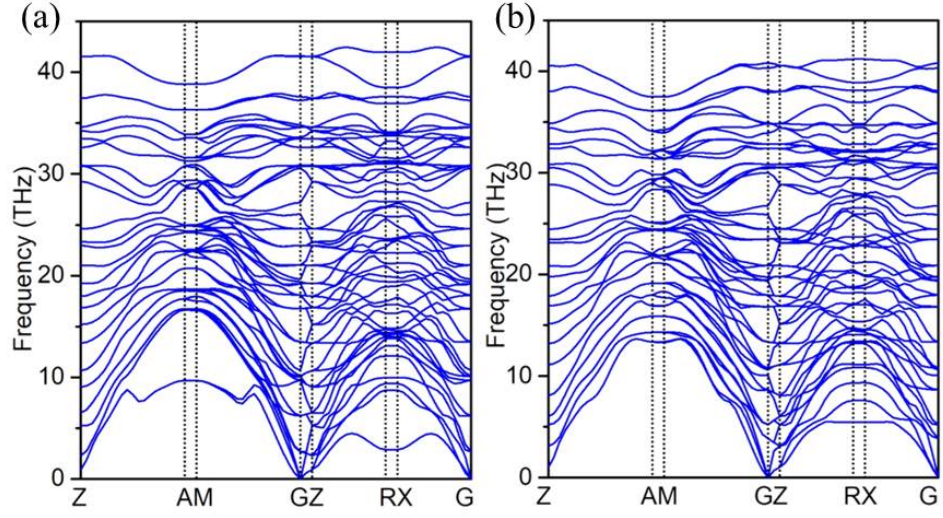
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**Fig. S1** Phonon dispersion of BN polymorphs.

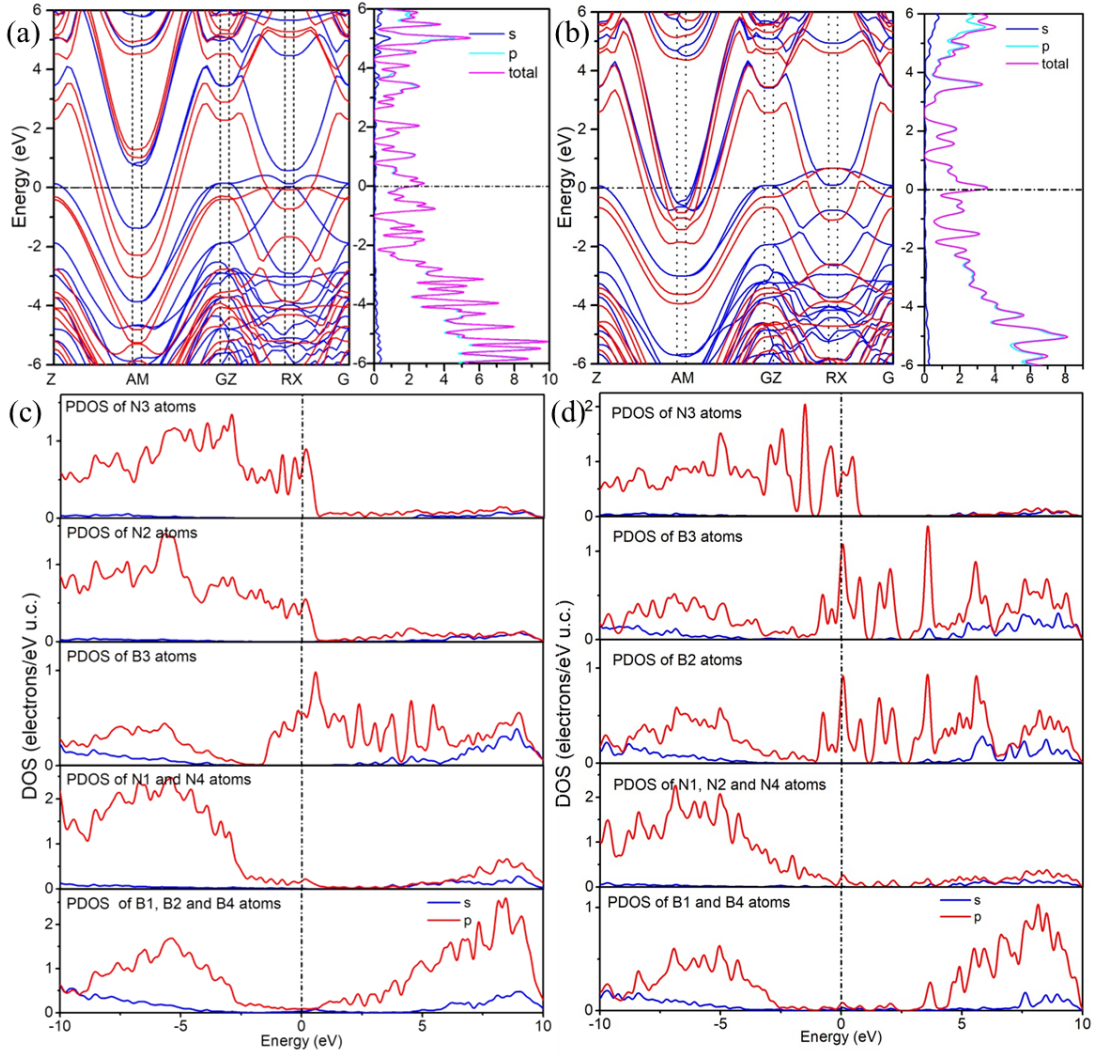
**Fig. S2** Electronic band structures and density of states of BN polymorphs.

**Table S1** Space group (S.G.), lattice parameters (Å), and atomic Wyckoff positions of  
BN polymorphs at ambient pressure.

**Table S2** Elastic constants  $C_{ij}$  (GPa), bulk modulus  $B$  (GPa), and shear modulus  $G$   
(GPa) of BN polymorphs.



**Fig. S1** Phonon dispersion of (a) B<sub>8</sub>N<sub>8</sub>-I (b) B<sub>8</sub>N<sub>8</sub>-II at zero pressure.



**Fig. S2** Electronic properties of onstructed metallic BN structures. (a) band structure of B<sub>8</sub>N<sub>8</sub>-I, (b) band structure of B<sub>8</sub>N<sub>8</sub>-II, (c) PDOS of B<sub>8</sub>N<sub>8</sub>-I, (d) PDOS of B<sub>8</sub>N<sub>8</sub>-II.

**Table S1.** Space group (S.G.), lattice parameters (Å), and atomic Wyckoff positions of BN polymorphs at ambient pressure.

Structure	S.G.	lattice parameters	Atomic positions
B <sub>8</sub> N <sub>8</sub> -I	<i>P42mc</i>	$a = b = 2.55 \text{ Å}, c = 15.86 \text{ Å};$ $\alpha = \beta = \gamma = 90^\circ$	B1 2a (0,0,0.886), B2 2c (0,0.5,0.748), B3 2a (0,0,0.611); B4 2b (0.5,0.5,0.5); N1 2c (0.5,0,0.561); N2 2a (0,0,0.702); N3 2c (0,0.5,0.836); N4 2c (0.5,0,0.947)
B <sub>8</sub> N <sub>8</sub> -II	<i>P42mc</i>	$a = b = 2.55 \text{ Å}, c = 15.91 \text{ Å};$ $\alpha = \beta = \gamma = 90^\circ$	B1 2c (0.5,0,0.561); B2 2a (0,0,0.702); B3 2c (0,0.5,0.836); B4 2c (0.5,0,0.947); N1 2a (0,0,0.886), N2 2c (0,0.5,0.748), N3 2a (0,0,0.611); N4 2b (0.5,0.5,0.5);

**Table S2.** Elastic constants  $C_{ij}$  (GPa), bulk modulus  $B$  (GPa), and shear modulus  $G$  (GPa) of BN polymorphs.

Structure	$C_{11}$	$C_{33}$	$C_{44}$	$C_{66}$	$C_{12}$	$C_{13}$	$B$	$G$
B <sub>8</sub> N <sub>8</sub> -I	731.4	916.7	135.5	113.4	37.2	138.0	329.6	192.1
B <sub>8</sub> N <sub>8</sub> -II	695.7	898.8	122.5	109.7	52.2	149.6	327.4	178.9