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


# Supplementary information for the manuscript "Multiporous $sp^2$-hybridized boron nitride (d-BN): Stability, mechanical properties, lattice thermal conductivity and promising application in energy storage."

Yingxiang Cai*[a], Li Zeng[a], Yu Zhang[a] and Xuechun Xu[a]

[a] Department of Physics, NanChang University, Jiangxi, Nanchang 330031, P.R. China.

E-mail: yingxiangcai@ncu.edu.cn

**1: Supporting Figures.**

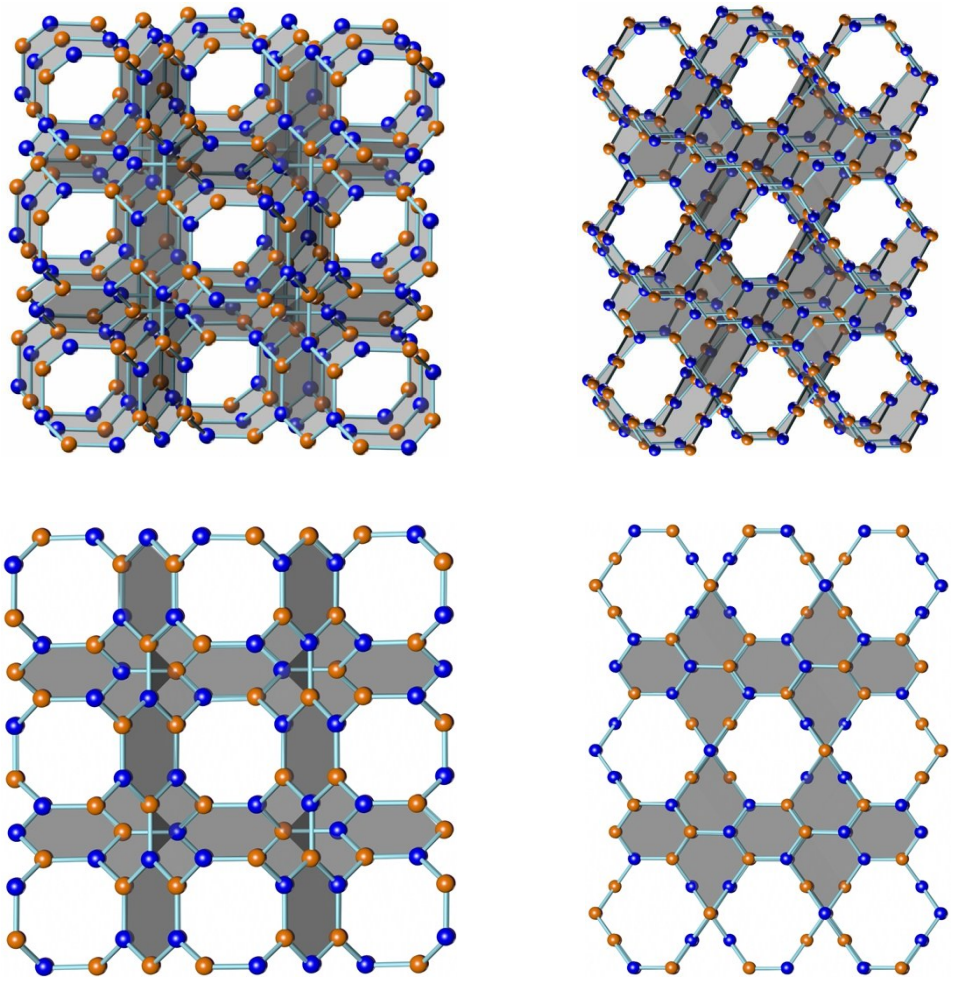

Fig. S1. The 3D models of d-BN viewed along [100] (left) and [110] (right) directions. The pores are rendered using grey surfaces.

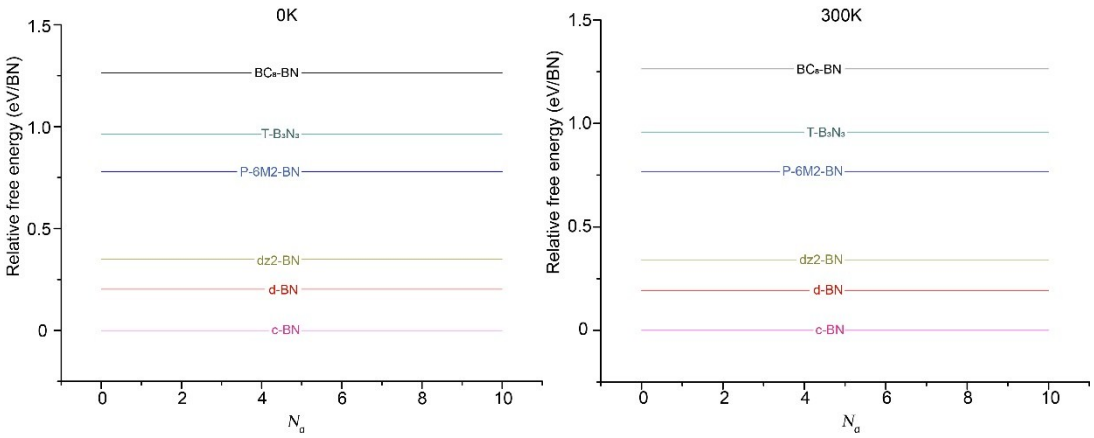


Fig. S2. The relative free energy of $BC_8$-BN, T-$B_3N_3$, P-6M2-BN, dz2-BN, d-BN and c-BN at 0K (left) and 300K (right). Here, the free energy of c-BN is taken as a reference.

Along [100]:

Along [110]:

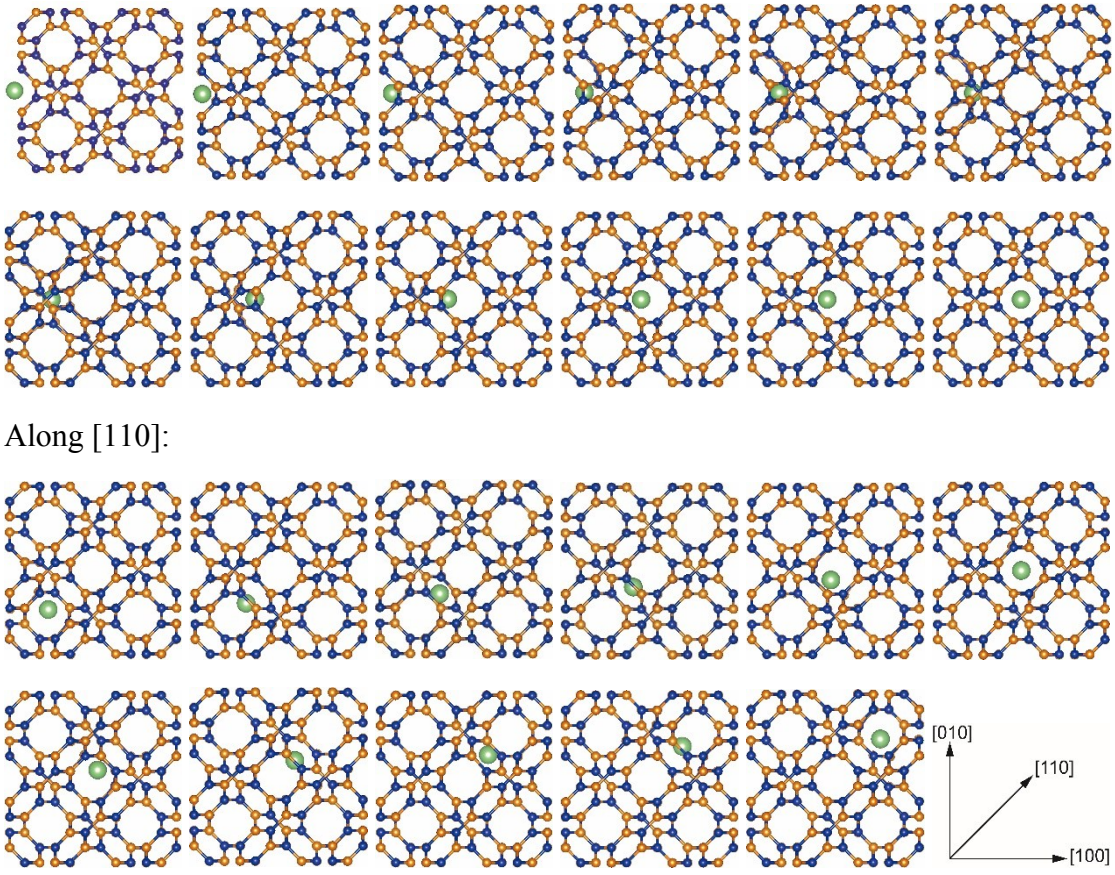


Fig. S3. The diffusion process of Li along [100] and [110] directions of the d-BN.

**2: Details of thermal conductivity modeling**.[1]

For the Hamiltonian **H** , the expansion is defined as:

$$\mathbf{H} = \Phi_0 + \mathbf{T} + \mathbf{H}_2 + \mathbf{H}_3 + \ldots$$

Where $\Phi_0$ is constant potential, **T** is kinetic energy, and $\mathbf{H}_n$ are n-body crystal potential terms. The harmonic Hamiltonian can be written as $\mathbf{H}_H = \mathbf{T} + \mathbf{H}_2$, and this harmonic part can be calculated as a sum of harmonic oscillators:

$$\mathbf{H}_H = \sum_{qj} \hbar\omega_{qj}\left(\frac{1}{2} + \hat{a}^{\dagger}_{qj}\hat{a}_{qj}\right)$$

and the third-order potential can be written as a sum of three-phonon collisions:

$$\mathbf{H}_H = \sum_{\lambda\lambda'\lambda''} \Phi_{\lambda\lambda'\lambda''}(\hat{a}_{\lambda} + \hat{a}^{\dagger}_{-\lambda})(\hat{a}_{\lambda'} + \hat{a}^{\dagger}_{-\lambda'})(\hat{a}_{\lambda''} + \hat{a}^{\dagger}_{-\lambda''})$$

Where $\hat{a}^{\dagger}_{-\lambda}$ and $\hat{a}_{\lambda}$ are the phonon creation and annihilation, and $\Phi_{\lambda\lambda'\lambda''}$ is the strength of interaction between the three phonon λ, λ′, λ″ involved in the scattering. As the imaginary part of the self-energy, $\Gamma_\lambda(\omega)$ can be computed up to second order in $\mathbf{H}_3$ using many-body perturbation theory:

$$\Gamma_{\lambda}(\omega) = \frac{18\pi}{\hbar^2}\sum_{\lambda'\lambda''} |\Phi_{-\lambda\lambda'\lambda''}|^2 \{\left(n_{\lambda'} + n_{\lambda''} + 1\right)\delta\left(\omega - \omega_{\lambda'} - \omega_{\lambda''}\right) + \left(n_{\lambda'} - n_{\lambda''}\right)\left[\delta($$

}

where $n_\lambda$ is the phonon occupation number at the equilibrium. $2\Gamma_\lambda(\omega)$ is the phonon linewidth of the phonon mode λ and its reciprocal is known as the phonon lifetime:

$$\tau_{\lambda} = \frac{1}{2\Gamma_{\lambda}(\omega_{\lambda})}$$

When the linearized phonon Boltzmann equation (LBTE) is solved under the single-mode relaxation-time (SMRT) method, the lattice thermal conductivity tensor can be written in a closed form:

$$\kappa = \frac{1}{NV_0}\sum_{\lambda} C_\lambda v_\lambda \otimes v_\lambda \tau_\lambda^{SMRT}$$

**3: The POSCAR files of optimized unit-cells for d-BN and other BN polymorphs including $BC_8$-BN, c-BN, cT8-BN, dz2-BN, Hexagonal-BN, Hp-BN, M-BN, P-6M2-BN and T-$B_3N_3$.**

**No.1** $BC_8$-BN

1.000000

4.524019 0.000000 0.000000

0.000000 4.524019 0.000000

0.000000 0.000000 4.524019

B N

8 8

Direct

0.840018 0.659982 0.340018

0.159982 0.340018 0.659982

0.659982 0.340018 0.840018

0.340018 0.659982 0.159982

0.159982 0.159982 0.159982

0.840018 0.840018 0.840018

0.340018 0.840018 0.659982

0.659982 0.159982 0.340018

0.347160 0.152840 0.847160

0.652840 0.847160 0.152840

0.152840 0.847160 0.347160

0.847160 0.152840 0.652840

0.652840 0.652840 0.652840

0.347160 0.347160 0.347160

0.847160 0.347160 0.152840

0.152840 0.652840 0.847160

**No.2** c-BN

1.000000

3.606645 0.000000 0.000000

0.000000 3.606645 0.000000

0.000000 0.000000 3.606645

B N

4 4

Direct

0.000000 0.000000 0.000000

0.000000 0.500000 0.500000

0.500000 0.000000 0.500000

0.500000 0.500000 0.000000

0.250000 0.250000 0.250000

0.750000 0.750000 0.250000

0.750000 0.250000 0.750000

0.250000 0.750000 0.750000

**No.3** cT8-BN

1.000000

6.069689 0.000000 0.000000

0.000000 6.069689 0.000000

0.000000 0.000000 3.731765

B N

8 8

Direct

0.250000 0.118162 0.375000

0.750000 0.881838 0.375000

0.118162 0.750000 0.625000

0.881838 0.250000 0.625000

0.381838 0.750000 0.125000

0.618162 0.250000 0.125000

0.750000 0.618162 0.875000

0.250000 0.381838 0.875000

0.250000 0.887572 0.375000

0.750000 0.112428 0.375000

0.887572 0.750000 0.625000

0.112428 0.250000 0.625000

0.612428 0.750000 0.125000

0.387572 0.250000 0.125000

0.750000 0.387572 0.875000

0.250000 0.612428 0.875000

**No.4** dz2-BN

1.000000

4.927142 0.000000 0.000000

0.000000 3.169118 0.000000

0.000000 0.000000 8.044761

B N

8 8

Direct

0.000000 0.000000 0.329530

0.500000 0.000000 0.329530

0.500000 0.500000 0.829530

0.000000 0.500000 0.829530

0.250000 0.875881 0.590830

0.750000 0.124119 0.590830

0.750000 0.375881 0.090830

0.250000 0.624119 0.090830

0.000000 0.000000 0.507471

0.500000 0.000000 0.507471

0.500000 0.500000 0.007471

0.000000 0.500000 0.007471

0.250000 0.625758 0.742170

0.750000 0.374242 0.742170

0.750000 0.125758 0.242170

0.250000 0.874242 0.242170

**No.5** Hexagonal-BN

1.000000

2.504705 -0.006297 0.000000

-1.257806 2.165989 -0.000000

-0.000000 0.000000 6.718220

B N

2 2

Direct

0.355190 0.644810 0.250000

0.644810 0.355190 0.750000

0.022659 0.977341 0.250000

0.977341 0.022659 0.750000

**No.6** Hp-BN

1.000000

2.596874 -0.000000 0.000000

-1.298437 2.248959 0.000000

0.000000 0.000000 5.801412

B N

3 3

Direct

0.500000 0.000000 0.000000

0.000000 0.500000 0.666667

0.500000 0.500000 0.333333

0.500000 0.500000 0.833333

0.500000 0.000000 0.500000

0.000000 0.500000 0.166667

**No.7** M-BN

1.000000

9.413113 0.000000 0.051964

0.000000 2.560476 0.000000

-0.480831 0.000000 4.158881

B N

8 8

Direct

0.423259 0.500000 0.135136

0.258873 0.500000 0.924287

0.923259 0.000000 0.135136

0.758873 0.000000 0.924287

0.245930 0.000000 0.407390

0.745930 0.500000 0.407390

0.535254 0.000000 0.659009

0.035254 0.500000 0.659009

0.536928 0.500000 0.892476

0.689680 0.500000 0.047025

0.036928 0.000000 0.892476

0.189680 0.000000 0.047025

0.419907 0.000000 0.364211

0.919907 0.500000 0.364211

0.698280 0.000000 0.570467

0.198280 0.500000 0.570466

**No.8** P-6M2-BN

1.000000

6.353346 0.000000 0.000000

-3.176673 5.502159 0.000000

0.000000 0.000000 2.500311

B N

4 4

Direct

0.866945 0.133055 0.000000

0.866945 0.733889 0.000000

0.266111 0.133055 0.000000

0.666667 0.333333 0.500000

0.801415 0.198585 0.500000

0.801415 0.602829 0.500000

0.397171 0.198585 0.500000

0.000000 0.000000 0.000000

**No.9** T-$B_3N_3$

1.000000

2.621788 0.000000 0.000000

0.000000 2.621788 0.000000

0.000000 0.000000 6.092797

B N

3 3

Direct

0.000000 0.500000 0.860162

0.500000 0.000000 0.139838

0.500000 0.500000 0.500000

0.500000 0.500000 0.000000

0.000000 0.500000 0.638170

0.500000 0.000000 0.361830

**No.10** d-BN

1.000000

12.293114 0.000000 0.000000

0.000000 12.293114 0.000000

0.000000 0.000000 12.293114

N B

96 96

Direct

0.125000 0.292579 0.457421

0.375000 0.207421 0.457421

0.375000 0.292579 0.042579

0.125000 0.207421 0.042579

0.457421 0.125000 0.292579

0.457421 0.375000 0.207421

0.042579 0.375000 0.292579

0.042579 0.125000 0.207421

0.292579 0.457421 0.125000

0.207421 0.457421 0.375000

0.292579 0.042579 0.375000

0.207421 0.042579 0.125000

0.625000 0.457421 0.292579

0.875000 0.042579 0.292579

0.875000 0.457421 0.207421

0.625000 0.042579 0.207421

0.792579 0.125000 0.457421

0.792579 0.375000 0.042579

0.707421 0.375000 0.457421

0.707421 0.125000 0.042579

0.957421 0.292579 0.125000

0.542579 0.292579 0.375000

0.957421 0.207421 0.375000

0.542579 0.207421 0.125000

0.125000 0.957421 0.292579

0.375000 0.542579 0.292579

0.375000 0.957421 0.207421

0.125000 0.542579 0.207421

0.292579 0.625000 0.457421

0.292579 0.875000 0.042579

0.207421 0.875000 0.457421

0.207421 0.625000 0.042579

0.457421 0.792579 0.125000

0.042579 0.792579 0.375000

0.457421 0.707421 0.375000

0.042579 0.707421 0.125000

0.625000 0.792579 0.457421

0.875000 0.707421 0.457421

0.875000 0.792579 0.042579

0.625000 0.707421 0.042579

0.957421 0.625000 0.292579

0.957421 0.875000 0.207421

0.542579 0.875000 0.292579

0.542579 0.625000 0.207421

0.792579 0.957421 0.125000

0.707421 0.957421 0.375000

0.792579 0.542579 0.375000

0.707421 0.542579 0.125000

0.125000 0.457421 0.792579

0.375000 0.042579 0.792579

0.375000 0.457421 0.707421

0.125000 0.042579 0.707421

0.292579 0.125000 0.957421

0.292579 0.375000 0.542579

0.207421 0.375000 0.957421

0.207421 0.125000 0.542579

0.457421 0.292579 0.625000

0.042579 0.292579 0.875000

0.457421 0.207421 0.875000

0.042579 0.207421 0.625000

0.625000 0.292579 0.957421

0.875000 0.207421 0.957421

0.875000 0.292579 0.542579

0.625000 0.207421 0.542579

0.957421 0.125000 0.792579

0.957421 0.375000 0.707421

0.542579 0.375000 0.792579

0.542579 0.125000 0.707421

0.792579 0.457421 0.625000

0.707421 0.457421 0.875000

0.792579 0.042579 0.875000

0.707421 0.042579 0.625000

0.125000 0.792579 0.957421

0.375000 0.707421 0.957421

0.375000 0.792579 0.542579

0.125000 0.707421 0.542579

0.457421 0.625000 0.792579

0.457421 0.875000 0.707421

0.042579 0.875000 0.792579

0.042579 0.625000 0.707421

0.292579 0.957421 0.625000

0.207421 0.957421 0.875000

0.292579 0.542579 0.875000

0.207421 0.542579 0.625000

0.625000 0.957421 0.792579

0.875000 0.542579 0.792579

0.875000 0.957421 0.707421

0.625000 0.542579 0.707421

0.792579 0.625000 0.957421

0.792579 0.875000 0.542579

0.707421 0.875000 0.957421

0.707421 0.625000 0.542579

0.957421 0.792579 0.625000

0.542579 0.792579 0.875000

0.957421 0.707421 0.875000

0.542579 0.707421 0.625000

0.125000 0.457475 0.292525

0.375000 0.042525 0.292525

0.375000 0.457475 0.207475

0.125000 0.042525 0.207475

0.292525 0.125000 0.457475

0.292525 0.375000 0.042525

0.207475 0.375000 0.457475

0.207475 0.125000 0.042525

0.457475 0.292525 0.125000

0.042525 0.292525 0.375000

0.457475 0.207475 0.375000

0.042525 0.207475 0.125000

0.625000 0.292525 0.457475

0.875000 0.207475 0.457475

0.875000 0.292525 0.042525

0.625000 0.207475 0.042525

0.957475 0.125000 0.292525

0.957475 0.375000 0.207475

0.542525 0.375000 0.292525

0.542525 0.125000 0.207475

0.792525 0.457475 0.125000

0.707475 0.457475 0.375000

0.792525 0.042525 0.375000

0.707475 0.042525 0.125000

0.125000 0.792525 0.457475

0.375000 0.707475 0.457475

0.375000 0.792525 0.042525

0.125000 0.707475 0.042525

0.457475 0.625000 0.292525

0.457475 0.875000 0.207475

0.042525 0.875000 0.292525

0.042525 0.625000 0.207475

0.292525 0.957475 0.125000

0.207475 0.957475 0.375000

0.292525 0.542525 0.375000

0.207475 0.542525 0.125000

0.625000 0.957475 0.292525

0.875000 0.542525 0.292525

0.875000 0.957475 0.207475

0.625000 0.542525 0.207475

0.792525 0.625000 0.457475

0.792525 0.875000 0.042525

0.707475 0.875000 0.457475

0.707475 0.625000 0.042525

0.957475 0.792525 0.125000

0.542525 0.792525 0.375000

0.957475 0.707475 0.375000

0.542525 0.707475 0.125000

0.125000 0.292525 0.957475

0.375000 0.207475 0.957475

0.375000 0.292525 0.542525

0.125000 0.207475 0.542525

0.457475 0.125000 0.792525

0.457475 0.375000 0.707475

0.042525 0.375000 0.792525

0.042525 0.125000 0.707475

0.292525 0.457475 0.625000

0.207475 0.457475 0.875000

0.292525 0.042525 0.875000

0.207475 0.042525 0.625000

0.625000 0.457475 0.792525

0.875000 0.042525 0.792525

0.875000 0.457475 0.707475

0.625000 0.042525 0.707475

0.792525 0.125000 0.957475

0.792525 0.375000 0.542525

0.707475 0.375000 0.957475

0.707475 0.125000 0.542525

0.957475 0.292525 0.625000

0.542525 0.292525 0.875000

0.957475 0.207475 0.875000

0.542525 0.207475 0.625000

0.125000 0.957475 0.792525

0.375000 0.542525 0.792525

0.375000 0.957475 0.707475

0.125000 0.542525 0.707475

0.292525 0.625000 0.957475

0.292525 0.875000 0.542525

0.207475 0.875000 0.957475

0.207475 0.625000 0.542525

0.457475 0.792525 0.625000

0.042525 0.792525 0.875000

0.457475 0.707475 0.875000

0.042525 0.707475 0.625000

0.625000 0.792525 0.957475

0.875000 0.707475 0.957475

0.875000 0.792525 0.542525

0.625000 0.707475 0.542525

0.957475 0.625000 0.792525

0.957475 0.875000 0.707475

0.542525 0.875000 0.792525

0.542525 0.625000 0.707475

0.792525 0.957475 0.625000

0.707475 0.957475 0.875000

0.792525 0.542525 0.875000

0.707475 0.542525 0.625000

**Reference**


1. A. Togo and I. Tanaka, Scr. Mater., 2015, 108, 1–5.
2. A. Togo, L. Chaput and I. Tanaka, Phys. Rev. B, 2015, 91, 094306.