Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supplementary information for

The intrinsic thermal transport property of biphenylene network and the influence of hydrogenation: A first-principles study

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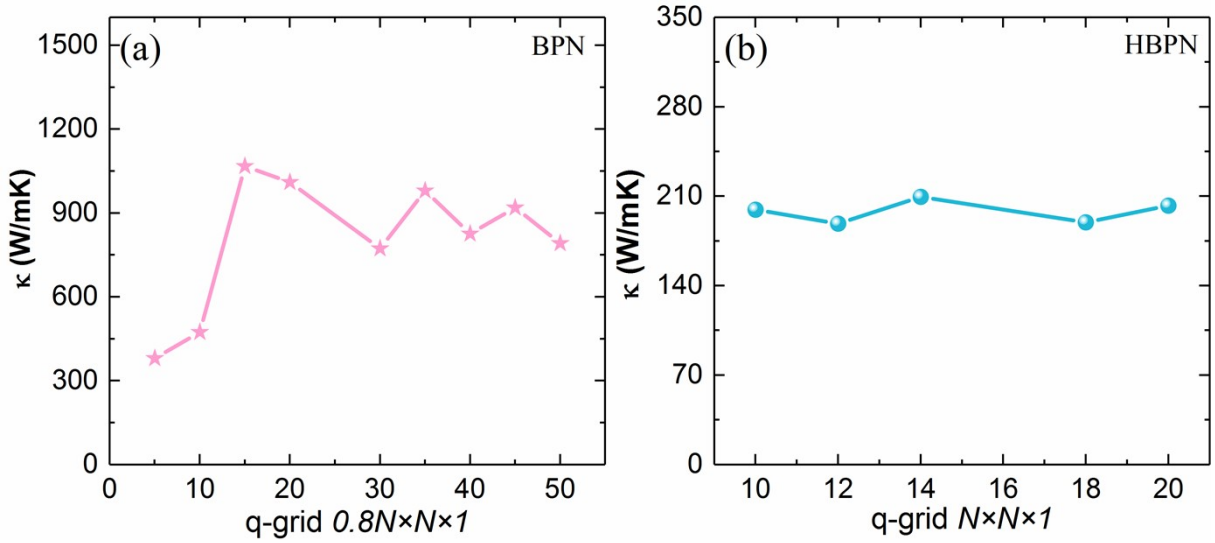

Figure S1. The averaged thermal conductivity (κ) of (a) BPN and (b) HBPN as a function q-grid with iterative method include three-phonon scattering.

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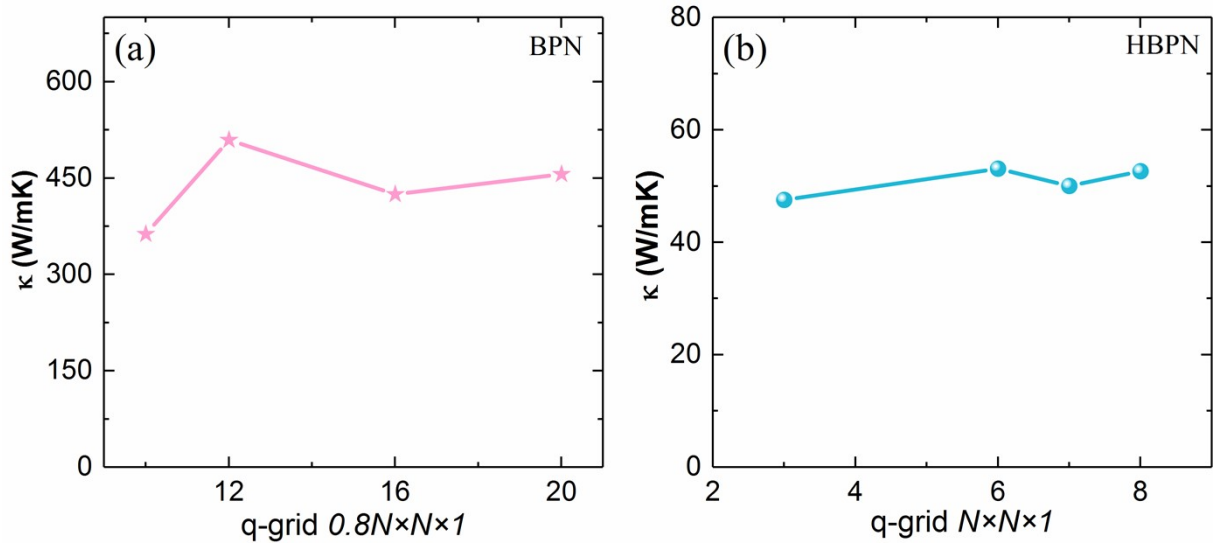

Figure S2. The averaged thermal conductivity (κ) of (a) BPN and (b) HBPN as a function q-grid with relaxation time approximation method include four-phonon scattering.

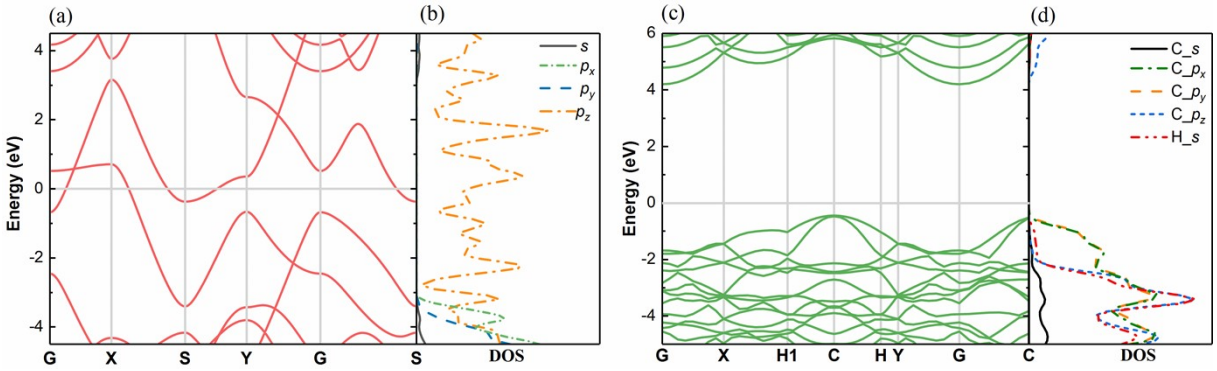

Figure S3. Electron energy band structure and corresponding partial density of states (DOS) of (a, b) BPN and (c, b) HBPN.

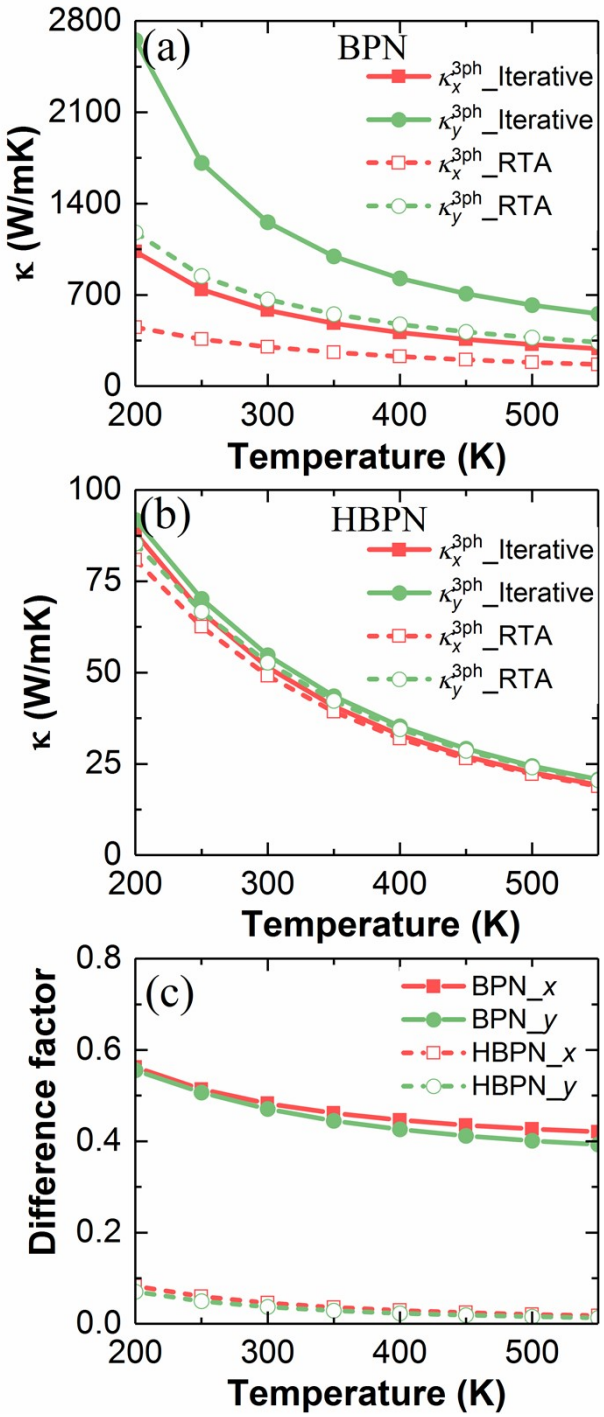

Figure S4. Lattice thermal conductivity (κ) versus temperature for (a) BPN and (b) HBPN with both iterative and RTA methods. Only the three-phonon scattering is included. (C) Difference factor ($1-\kappa_{RTA}^{3ph}/\kappa_{\text{Iterative}}^{3ph}$) as a function of temperature.

Table S1. Calculated independent elastic constants of BPN and HBPN (C_{11}, C_{22}, C_{12} and C_{66} in unit of N/m) and the corresponding Young's modulus (Y in unit of N/m) along the *x* and *y* direction.

Material	$\mathbf{C_{11}}$	$\mathbf{C_{22}}$	$\mathbf{C_{12}}$	$\mathbf{C_{66}}$	$\mathbf{Y_x}$	$\mathbf{Y_y}$
BPN	242.29	305.88	77.97	81.27	22.42	280.79
HBPN	142.35	210.87	15.15	61.53	141.26	209.24

Table S2. Trace of harmonic second order force constant (2^{nd} FC)

Material		**BPN**			**HBPN**	
Distance (Å)	3	4	5	3	4	5
Trace of 2^{nd} FC (eV/Å^2)	0.496	0.078	0.163	0.128	0.026	0.050