Supplementary information

A Theoretical Calculation Guided Strategy for Designing Energetic Composite Materials with Enhanced Thermal Conductivity by Adjusting Interfacial Interactions

Jialu Guan[a], Junqing Lv[a], Wei Chen[a], Mai Zhang[a], Yanze Liu[a], Guanchen Dong[a], Bowei Gao[a], Weihua Zhu[a], Guangcheng Yang[d], Qiong Wu[c,]*, Linghua Tan[b,]*

[a]*School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China*

[b]*School of Safety Science and Engineering, Nanjing University of Science and Technology, Nanjing 210094, China*

[c]*School of Materials Science and Engineering, Jiangsu Key Laboratory of Advanced Structural Materials and Application Technology, Nanjing Institute of Technology, Nanjing 211167, China*

[d]*Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang 621022, Sichuan, China.*

#Jialu Guan and Junqing Lv contributed equally to this paper;

*Corresponding author: Linghua Tan, and Qiong Wu;

Email address: tanlh@njust.edu.cn (Linghua Tan), and qwunjit@163.com (Qiong Wu)

1. Sample LAMMPS Input Decks for the Force Field of the h-BNNS/HMX System

In this simulation system, the correspondence between atom types and atom IDs is defined as follows:

Types 1 through 5 correspond to atoms in the HMX molecule. Specifically, Type 1 represents hydrogen atom; Type 2 represents the nitrogen atom on the nitro group; Type 3 represents the nitrogen atom on the eight-membered ring; Type 4 represents oxygen atom; and Type 5 represents carbon atom.

Types 6 and 7 correspond to atoms on the h-BNNS, where Type 6 represents nitrogen atom and Type 7 represents boron atom.

Types 8 through 11 correspond to atoms on the h-BNNS-OH, where Type 8 represents hydrogen atom, Type 9 represents boron atom, Type 10 represents nitrogen atom and Type 11 represents oxygen atom.

This assignment ensures a clear distinction between the HMX and BNNS components when assigning force field parameters.

```
bond_style        harmonic
angle_style       harmonic
dihedral_style    hybrid harmonic multi/harmonic
improper_style    harmonic
pair_style        hybrid/overlay buck/coul/long 11.0 lj/cut 11.0 tersoff

bond_coeff        1   560.0000    1.2300
bond_coeff        2   495.8500    1.3600
bond_coeff        3   336.0500    1.4400
bond_coeff        4   340.0500    1.0900
bond_coeff        5   727.2177    1.467
bond_coeff        6   508.6717    0.993

angle_coeff       1    62.5000   120.9170
angle_coeff       2    62.5000   107.4525
angle_coeff       3    65.0000    95.8157
angle_coeff       4    35.0000   105.5961
angle_coeff       5    43.2000   107.0056
angle_coeff       6    38.5000   108.5067
angle_coeff       7    35.0000   110.5178

dihedral_coeff    1   multi/harmonic   8.450   0.000 -5.290   0.000 -3.160
dihedral_coeff    2   harmonic        -0.080 -1        3
dihedral_coeff    3   multi/harmonic   0.095 -1.485   1.610 -0.220   0.000

improper_coeff    1     4.0000    0.0000
improper_coeff    2    44.6500    0.0000

pair_coeff        * * tersoff BNC.tersoff NULL NULL NULL NULL NULL N B
pair_coeff        1 1 buck/coul/long  2649.70     0.26737968    27.34544584
pair_coeff        1 1 lj/cut  0.0000125    3.20855615
pair_coeff        1 2 buck/coul/long   12695.88    0.26595745    116.9071639
pair_coeff        1 2 lj/cut   0.0000125    3.191489362
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pair_coeff          1 3 buck/coul/long   12695.88     0.26595745    116.9071639
pair_coeff          1 3 lj/cut       0.0000125        3.191489362
pair_coeff          1 4 buck/coul/long   14175.97     0.25634453    104.4176355
pair_coeff       1 4 lj/cut   0.0000125     3.076134325
pair_coeff          1 5 buck/coul/long       4320.00      0.29282577    138.1058732
pair_coeff       1 5 lj/cut  0.0000125      3.513909224
pair_coeff          2 2 buck/coul/long   60833.90     0.26455026    499.9488192
pair_coeff       2 2 lj/cut  0.0000125      3.174603175
pair_coeff          2 3 buck/coul/long   60833.90     0.26455026    499.9488192
pair_coeff          2 3 lj/cut       0.0000125        3.174603175
pair_coeff          2 4 buck/coul/long   67925.95     0.25503698    446.5589156
pair_coeff       2 4 lj/cut   0.0000125     3.060443764
pair_coeff          2 5 buck/coul/long   30183.57     0.29112082    565.939114
pair_coeff       2 5 lj/cut  0.0000125      3.493449782
pair_coeff          3 3 buck/coul/long   60833.90     0.26455026    499.9488192
pair_coeff       3 3 lj/cut   0.0000125     3.174603175
pair_coeff          3 4 buck/coul/long   67925.95     0.25503698    446.5589156
pair_coeff       3 4 lj/cut  0.0000125      3.060443764
pair_coeff          3 5 buck/coul/long   30183.57     0.29112082    565.939114
pair_coeff       3 5 lj/cut   0.0000125     3.493449782
pair_coeff          4 4 buck/coul/long   75844.80     0.24612355    398.8668123
pair_coeff       4 4 lj/cut  0.0000125      2.953482648
pair_coeff          4 5 buck/coul/long   33702.40     0.27964206    505.5286042
pair_coeff       4 5 lj/cut  0.0000125      3.355704698
pair_coeff          5 5 buck/coul/long   14976.00     0.32362460    640.6284832
pair_coeff       5 5 lj/cut   0.0000125     3.883495146

special_bonds    lj/coul 0.0 0.0 1.0 dihedral yes

pair_coeff    7    5    lj/cut    0.137477271   3.965303645
pair_coeff    7    1    lj/cut    0.088994382   3.432715834
pair_coeff    7    4    lj/cut    0.18734994    3.780277768
pair_coeff    7    2    lj/cut    0.181493802   3.885209261
pair_coeff    7    3    lj/cut    0.181493802   3.885209261

pair_coeff    6    5    lj/cut    0.138618181   3.773214412
pair_coeff    6    1    lj/cut    0.089732937   3.266426488
pair_coeff    6    4    lj/cut    0.188904738   3.597151651
pair_coeff    6    2    lj/cut    0.183     3.697
pair_coeff    6    3    lj/cut    0.183     3.697

pair_coeff    11   11   lj/cut    0.195     3.5
pair_coeff    8    8    lj/cut    0.044     2.886
pair_coeff    11   8    lj/cut    0.092628289   3.178207042
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pair_coeff	11	9	lj/cut	0.18734994	3.780277768
pair_coeff	8	9	lj/cut	0.088994382	3.432715834
pair_coeff	11	10	lj/cut	0.188904738	3.597151651
pair_coeff	8	10	lj/cut	0.089732937	3.266426488

pair_coeff	11	5	lj/cut	0.14309088	3.671307669
pair_coeff	11	1	lj/cut	0.092628289	3.178207042
pair_coeff	11	4	lj/cut	0.195	3.5
pair_coeff	11	2	lj/cut	0.188904738	3.597151651
pair_coeff	11	3	lj/cut	0.188904738	3.597151651
pair_coeff	8	5	lj/cut	0.067970582	3.333764539
pair_coeff	8	1	lj/cut	0.044	2.886
pair_coeff	8	4	lj/cut	0.092628289	3.178207042
pair_coeff	8	2	lj/cut	0.089732937	3.266426488
pair_coeff	8	3	lj/cut	0.089732937	3.266426488

pair_coeff	9	5	lj/cut	0.137477271	3.965303645
pair_coeff	9	1	lj/cut	0.088994382	3.432715834
pair_coeff	9	4	lj/cut	0.18734994	3.780277768
pair_coeff	9	2	lj/cut	0.181493802	3.885209261
pair_coeff	9	3	lj/cut	0.181493802	3.885209261
pair_coeff	10	5	lj/cut	0.138618181	3.773214412
pair_coeff	10	1	lj/cut	0.089732937	3.266426488
pair_coeff	10	4	lj/cut	0.188904738	3.597151651
pair_coeff	10	2	lj/cut	0.183	3.697
pair_coeff	10	3	lj/cut	0.183	3.697
```

Table S1 Thermal conductivity of HMX with different heat transfer lengths

Heat transfer lengths(nm)	Thermal conductivity(W/m·K)
5	0.210
10	0.552
20	0.739

Table S2 Comparison of lattice parameters of β-HMX from the SB force field, other computational methods, and experiments.

work	*a*	*b*	*c*
SB FF β-HMX	6.59536	10.41324	7.70733
Experimental[1]	6.54	11.05	8.7
%dev	0.84	-5.76	-11.41
GGA-PBE+TS[2]	6.63	11.22	8.82
%dev	-0.52	-7.19	-12.62
CASTEP[1]	6.61	10.98	8.75
%dev	-0.22	-5.16	-11.92

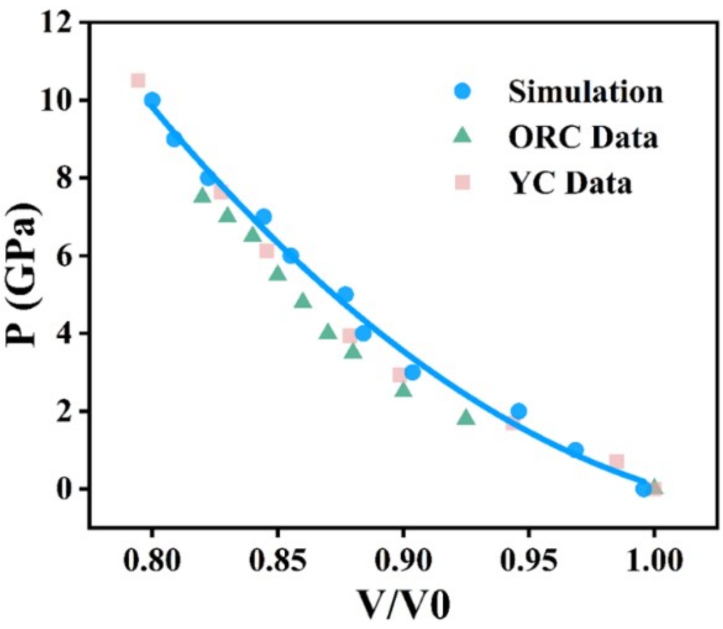

Figure S1. Pressure-volume (P-V) curve of the β-HMX lattice calculated using the Smith-Bharadwaj force field.[1]

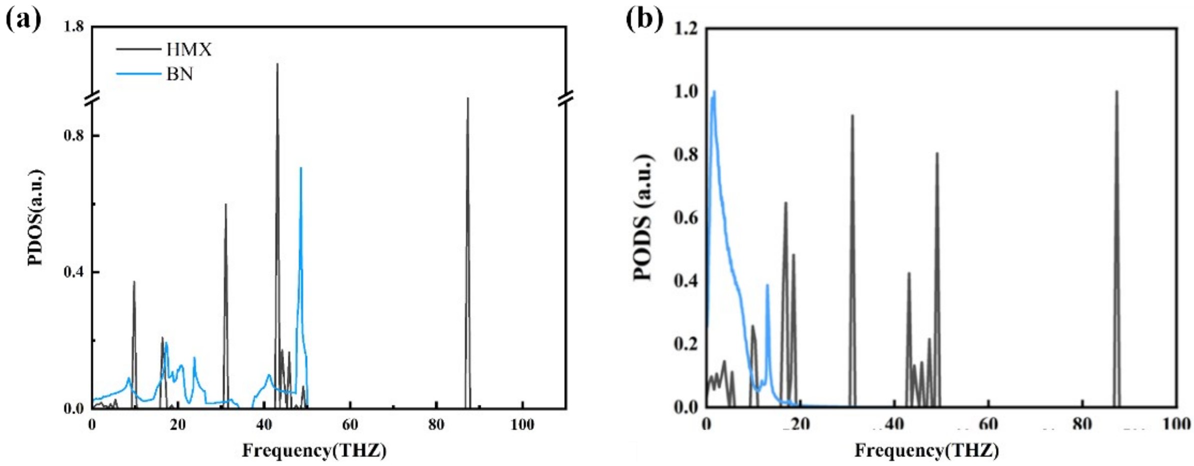

Figure S2 Phonon density of states of (a) h-BNNS/HMX and (b) h-BNNS-OH/HMX

Reference:

1. C.-S. Yoo and H. Cynn, *The Journal of Chemical Physics*, 1999, **111**, 10229-10235.
2. H. Qin, W. Zeng, F.-S. Liu, Y.-D. Gan, B. Tang, S.-H. Zhu and Q.-J. Liu, *Journal of Energetic Materials*, 2021, **39**, 125-169.