**Supplementary material**

**Temperature-dependent structural stability, mechanical strength, and thermodynamics of pyrite-type silicon pernitride**

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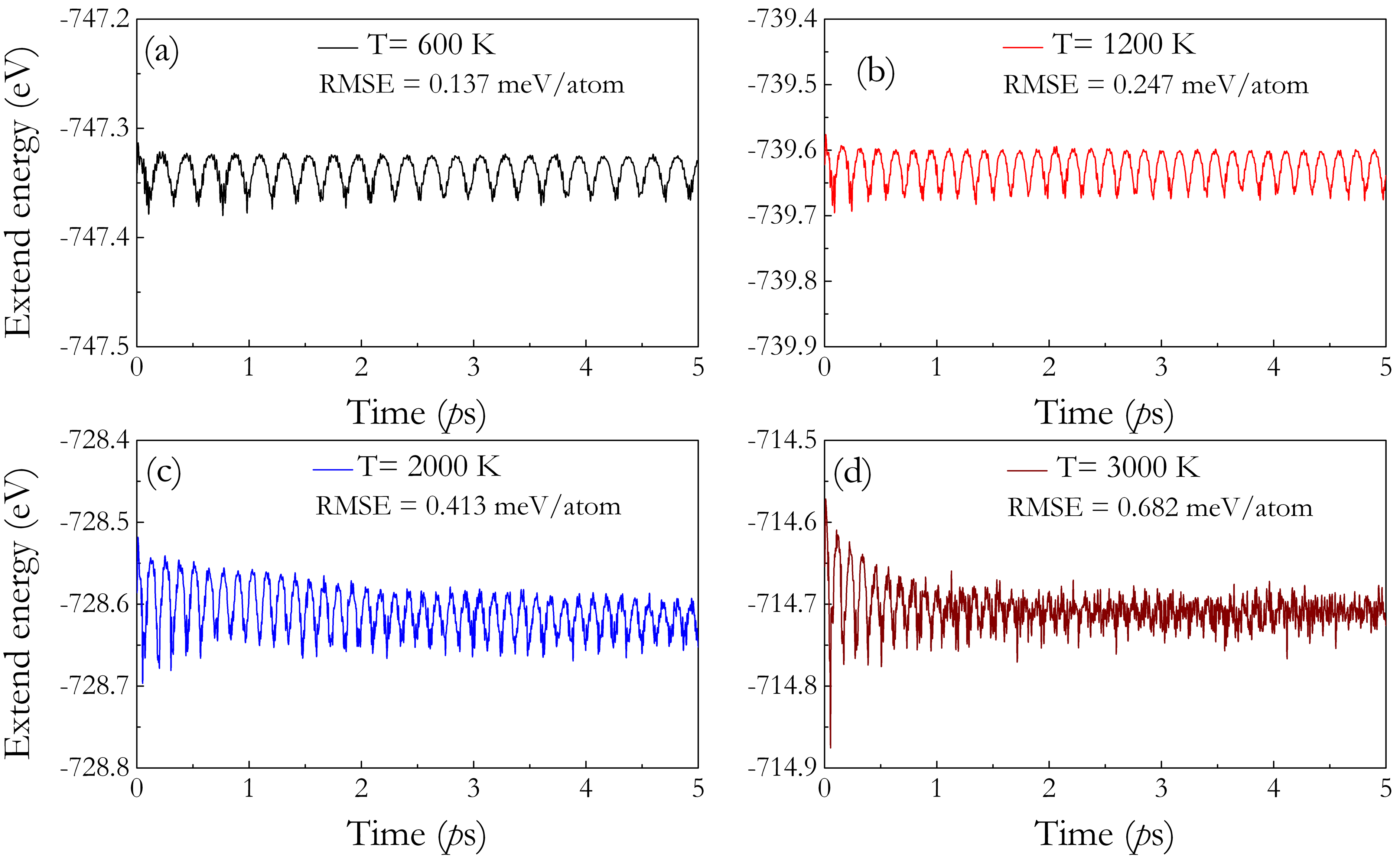
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**Table S1** AIMD tests of elastic constants *Cij*, the Hill bulk modulus *B*, shear modulus *G*, and Young's modulus *E* using different supercells for diamond and *p*-SiN2 (all in GPa).

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | *T* | Supercell | *K*-mesh | Source | *C*11 | *C*12 | *C*44 | *B* | *G* | *E* |
| Diamond | 1000 K | 2×2×2 | 4×4×4 | This work | 1006 | 120 | 520 | 417 | 488 | 1052 |
|  |  | 3×3×3 | 2×2×2 | This work | 997 | 113 | 531 | 408 | 493 | 1054 |
|  |  | 2×2×2 | 2×2×2 | Theory1 | 944 | 143 | 510 | 408 | 467 |  |
|  |  |  |  | Exp.2 | 1054.1 | 124.3 | 556.6 | 434.2 | 517.9 | 1111.7 |
| *p*-SiN2 | 1200 K | 2×2×2 | 4×4×4 | This work | 609 | 119 | 341 | 282 | 299 | 662 |
|  |  | 3×3×3 | 2×2×2 | This work | 606 | 121 | 342 | 283 | 298 | 661 |



**Fig. S1** AIMD NVT tests of extended system energy *vs.* time at different temperatures (using the Nosé-Hoover thermostat with 1 *f*s time step).



**Fig. S2** AIMD NPT tests of average stress–strain curves of *p*-SiN2 under ideal tensile strains along [001] direction at 900 K using two different supercells.



**Fig. S3** AIMD NPT simulations at 300, 600, 2000, and 3000 K for *p*-SiN2 under ambient conditions. Insets are the equilibrium structures after 30 *p*s.



**Fig. S4** High-temperature renormalized phonon spectra of *p*-SiN2 (a) and diamond (b).



**Fig. S5** Calculated N–N bond length versus ICOHP at various indentation shear strains alongdirection.

**References**

1 L. B. Wen, H. Wu, H. Sun and C. F. Chen, *Carbon*, 2019, **155**, 361−368.

2 E. S. Zouboulis, M. Grimsditch, A. K. Ramdas and S. Rodriguez, *Phys. Rev. B*, 1998, **57**,2889.

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