Electronic Supplementary Material (ESI) for RSC Advances.

Comparative DFT- and DFT-D-based molecular dynamics studies of pressure effects in crystalline 1,3,5-triamino-2,4,6-trinitrobenzene at room temperature

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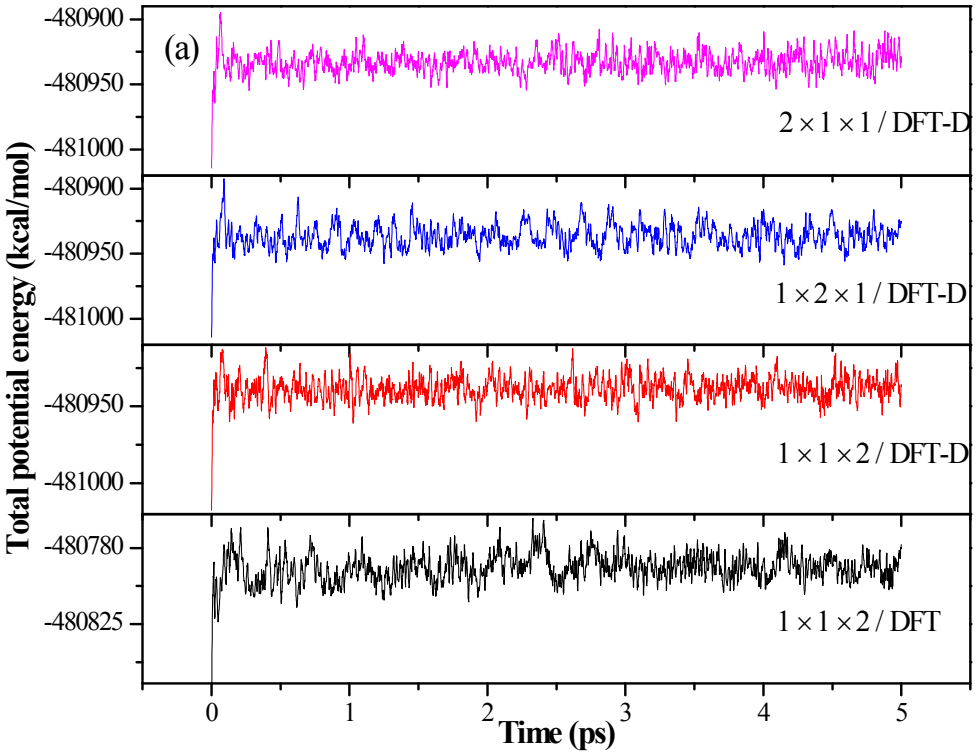

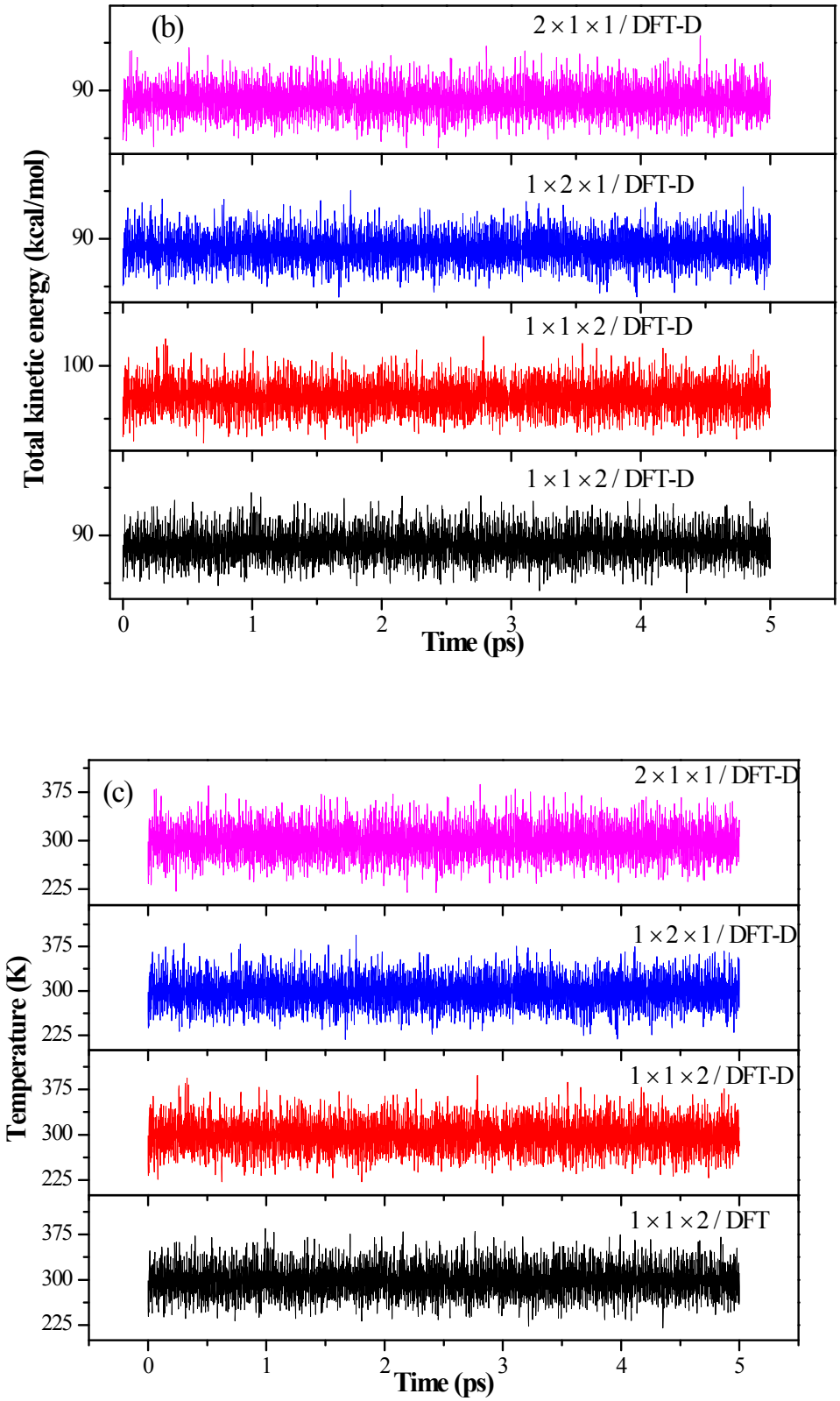

FIG. S1. The time dependences of total potential energy (a), total kinetic energy (b), and temperature (c) of TATB in the 5 ps of equilibration at 298.15 K by using *NVT* for all four systems (1 × 1 × 2 / DFT, 1 × 1 × 2 / DFT-D, 1 × 2 × 1 / DFT-D, and 2 × 1

× 1 / DFT-D).