

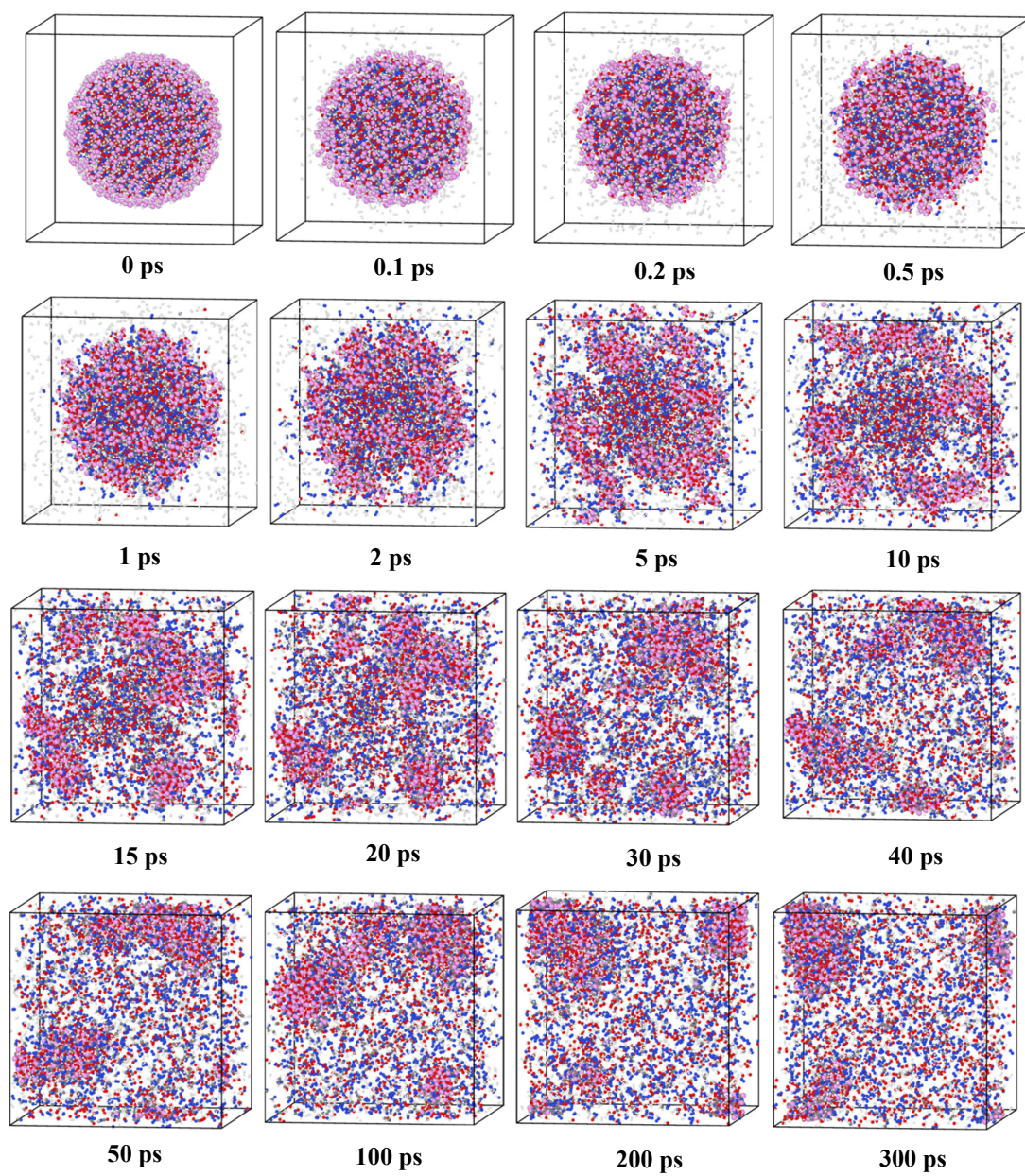
## Supplementary Information

**Thermal decomposition of core-shell structured RDX@AlH<sub>3</sub>, HMX@AlH<sub>3</sub>, and  
CL-20@AlH<sub>3</sub> nanoparticles: Reactive molecular dynamics simulations**

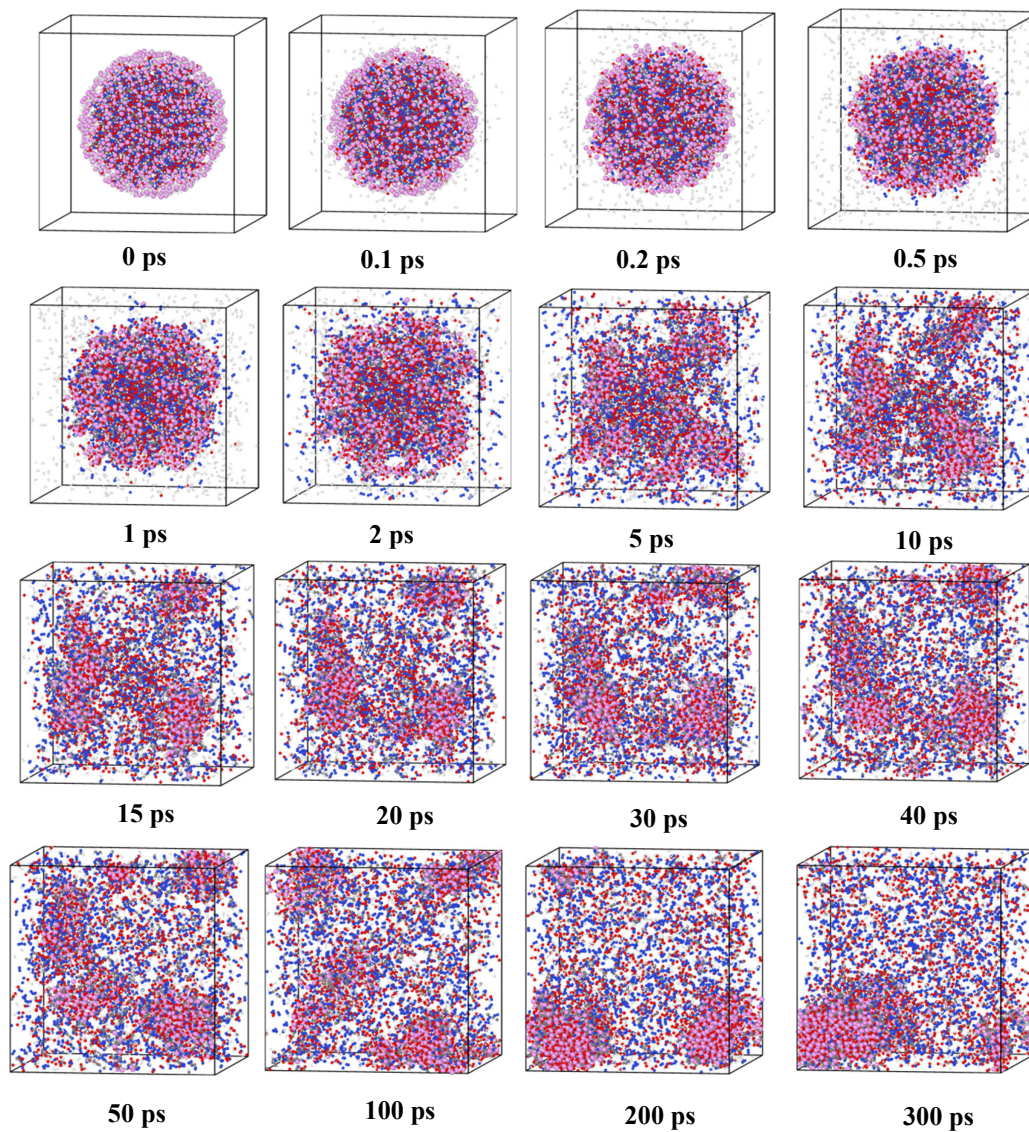
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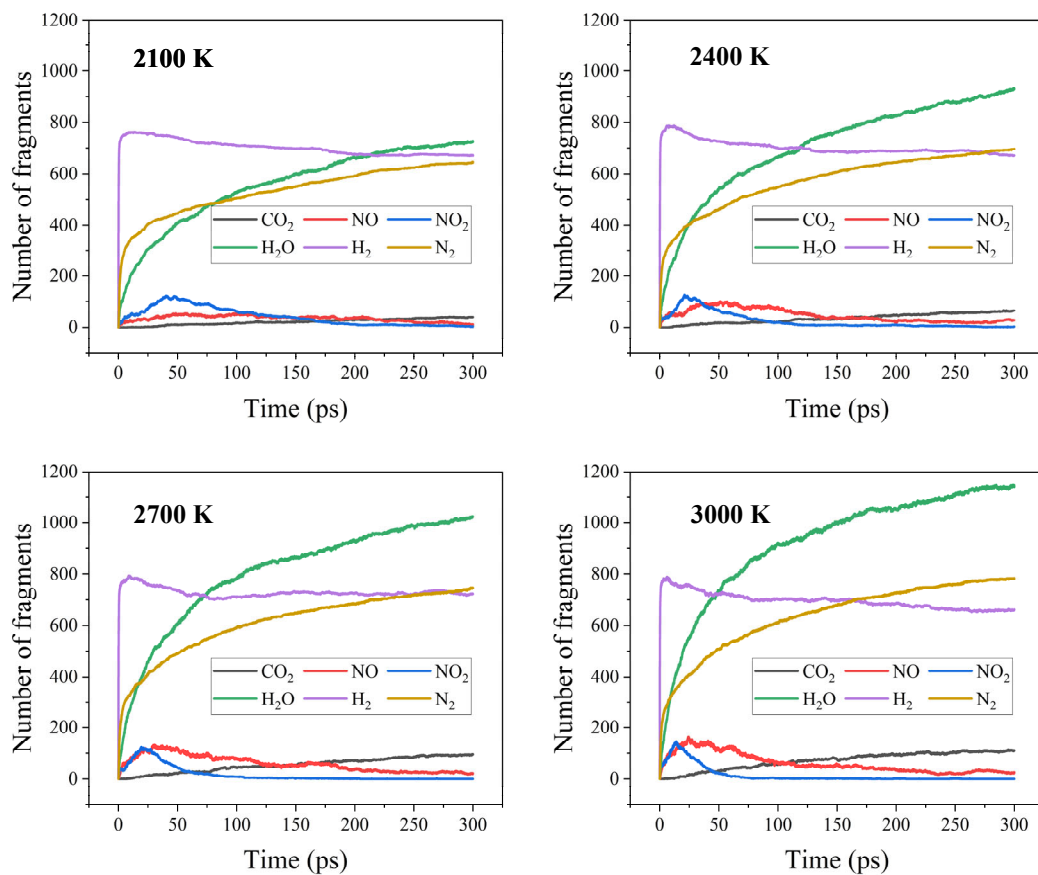


**Figure S1.** Snapshots of the morphology the decomposition process of the HMX@AlH<sub>3</sub> at 2400 K.

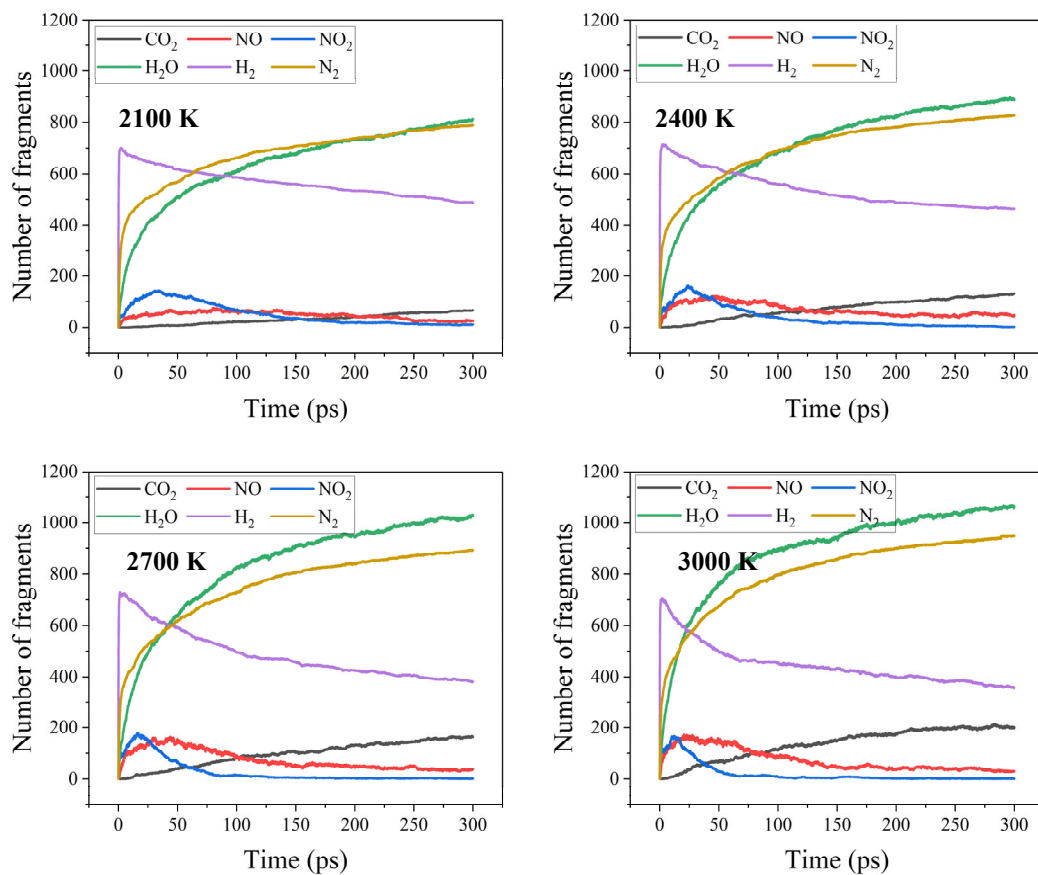


**Figure S2.** Snapshots of the morphology the decomposition process of the CL-20@AlH<sub>3</sub> at 2400 K.





**Figure S3.** Time evolution of the products of the  $\text{HMX@AlH}_3$  NP at 2100, 2400, 2700, and 3000 K.



**Figure S4.** Time evolution of the products of the CL-20@AlH<sub>3</sub> NP at 2100, 2400, 2700, and 3000 K.