Supplementary Information

Reaction Kinetics Properties of 1,3,5-Triamino-2,4,6-Trinitrobenzene: A DFTB Study for Thermal Decomposition

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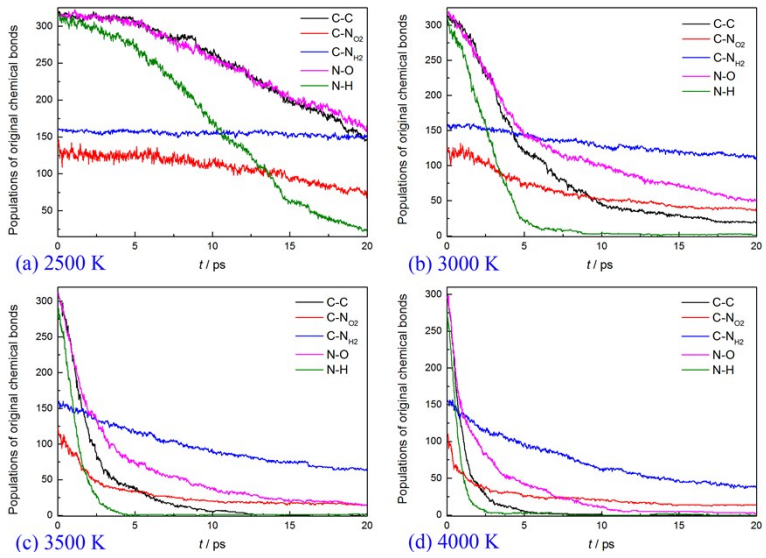

Fig. S1 Time evolutions of population of original chemical bonds involved in TATB thermal decomposition.

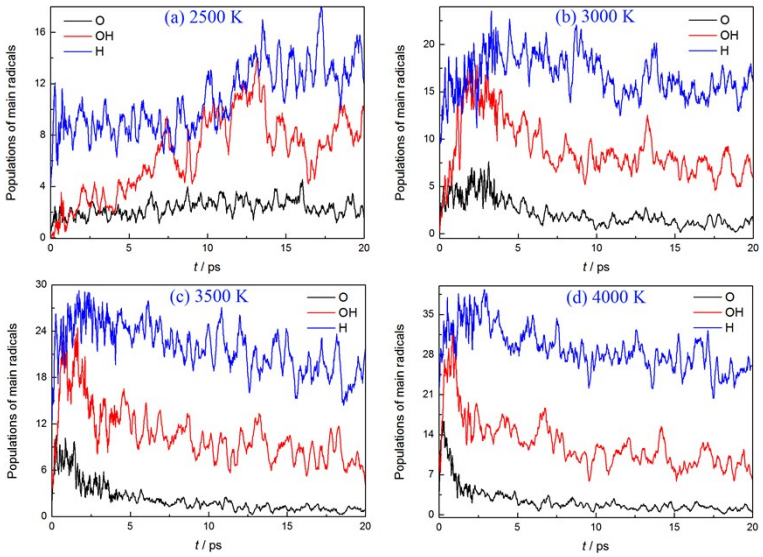

Fig. S2 Time evolutions of populations of the main radicals involved in TATB thermal decomposition.

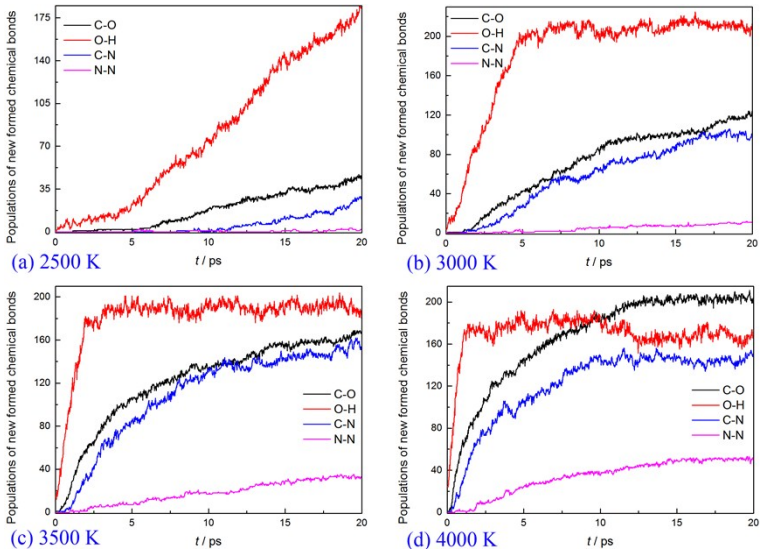

Fig. S3 Time evolutions of population of the main new-formed chemical bonds involved in TATB thermal decomposition.

Table S1. Parameters for the exponential fitting of the concentration evolutions of different chemical bonds.

T	Parameter	C-C	C-N	N-H	N-O	C-O*	O-H*	N-N*	C-N*
3000	**a** (mol·cm^{-3})	0.0447	0.0407	0.0445	0.0455	0.0247	0.0308	0.0246	0.0361
	k (x10^{12} s^{-1})	0.1686	0.0390	0.3535	0.1169	0.0608	0.3438	0.0039	0.0282
3500	**a** (mol·cm^{-3})	0.0445	0.0400	0.0403	0.0446	0.0233	0.0274	0.0116	0.0234
	k (x10^{12} s^{-1})	0.4529	0.8900	0.7732	0.2762	0.1982	0.9014	0.0308	0.1440
4000	**a** (mol·cm^{-3})	0.0429	0.0374	0.0394	0.0423	0.0292	0.0249	0.0081	0.0213
	k (x10^{12} s^{-1})	0.9691	0.1173	1.3844	0.4951	0.2621	1.9421	0.1347	0.2660

*new formed chemical bonds during TATB decomposition

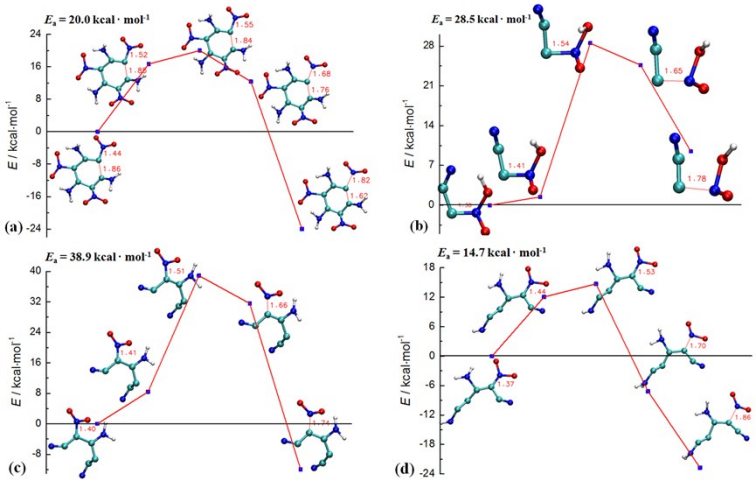

Fig. S4 Potential energy evolution during C-NO_2 bond dissociation (The fragment snapshots are drawn from the MD trajectory, which have no close interaction with other molecular fragments during the C-NO_2 bond fission.).