Influence of Al and Al_2O_3 Nanoparticles on the Thermal Decay of 1,3,5-Trinitro-1,3,5-triazinane (RDX): Reactive Molecular Dynamics Simulations

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Supporting Information

Table S1. Moment (t_D) at which RDX molecules undergo 50 % and 100 % decomposition.

T (K)	Model	t_D (ps)	
		50 %	100 %
1500	Al-RDX	1.85	125
	Al_2O_3-RDX	10.1	137.35
	Void-RDX	26.95	197.45
	RDX	29.9	189.5
2000	Al-RDX	0.72	47.8
	Al_2O_3-RDX	3.45	36.75
	Void-RDX	4.3	37.7
	RDX	3.3	22.85
2500	Al-RDX	0.78	26
	Al_2O_3-RDX	1.9	18.15
	Void-RDX	1.6	17.3
	RDX	0.95	8.85
3000	Al-RDX	0.77	14.8
	Al_2O_3-RDX	1.15	11.15
	Void-RDX	0.9	7.95
	RDX	0.7	3.8
3500	Al-RDX	0.67	9.6
	Al_2O_3-RDX	0.82	8.3
	Void-RDX	0.6	4.8
	RDX	0.46	2.4

Table S2. Total number (N) of molecules of the four models approaching the final equilibrium state at 2500 and 3500 K.

T (K)	Model	N
2500	Al-RDX	2424
	Al_2O_3-RDX	2692
	Void-RDX	2820
	RDX	3443
3500	Al-RDX	2544
	Al_2O_3-RDX	2875
	Void-RDX	2930
	RDX	3565

Video 1. ReaxFF-MD simulations of a single RDX molecule adsorbing onto the Al (001) surface at 1 K for 6 ps.

Video 2. ReaxFF-MD simulations of a single RDX molecule adsorbing onto the Al (001) surface at 5 K for 6 ps.

Video 3. ReaxFF-MD simulations of a single RDX molecule adsorbing onto the Al_2O_3 (0001) surface for 6 ps. Programmed heating was performed from 1 K to 1000 K within 6 ps.

Video 4. ReaxFF-MD simulations of a single RDX molecule adsorbing onto the Al_2O_3 (0001) surface at 300 K for 6 ps.

Video 5. ReaxFF-MD simulations of a single RDX molecule in vacuum at 2000 K for 10 ps.

Table S3. High frequent reactions leading to the final generation of N_2.

1500 K		3500 K	
Reactions	Freqs.	Reactions	Freqs.
CH_2ON_2 =>CH_2O +N_2	19	N_2O =>N_2 +O	48
$CH_2O_2N_2$ =>CH_2O +N_2 +O	10	$CHON_2$ =>CHO +N_2	43
N_2O =>N_2 +O	9	CH_2N_2 =>CH_2 +N_2	19
CH_3ON_2 =>CH_3O +N_2	9	CON_2 =>CO +N_2	18
$CH_2O_3N_3$=>CH_2O +N_2 +NO_2	5	HN_2 +O_2 =>HO_2 +N_2	18
$C_3H_6O_2N_6$ =>$C_3H_6O_2N_4$ +N_2	5	HON_2 =>HO +N_2	18
$CHON_4$ =>$CHON_2$ +N_2	5	CHO_2 +N_2 =>CO_2 +HN_2	17
$CHON_2$ =>CHO +N_2	5	CHON+CN_3 =>C_2HON_2+N_2	15
$CH_2O_2N_2$ =>CH_2O_2 +N_2	5	CHON +HN_2 =>CH_2ON +N_2	14
CH_2ON_3 =>CH_2ON +N_2	5	CO_2N_2 =>CO_2 +N_2	12
$C_3H_5O_3N_6$ =>$C_3H_5O_3N_4$ +N_2	5	HN_2 +HO =>H_2O +N_2	12

$CH_3O_2N_2 \Rightarrow CH_3O_2 + N_2$	4	$CON_3 \Rightarrow CON + N_2$	12
$HON_2 \Rightarrow HO + N_2$	4	$CH_2ON_3 \Rightarrow CH_2ON + N_2$	11
$CH_3O_2N_3 \Rightarrow CH_2ON + HO + N_2$	4	$H_2O + HN_2 \Rightarrow H_3O + N_2$	11
$C_2H_4O_2N_5 \Rightarrow C_2H_4O_2N_3 + N_2$	4	$CH_2ON_2 \Rightarrow CH_2O + N_2$	11
$C_2H_4O_2N_6 \Rightarrow C_2H_4O_2N_4 + N_2$	4	$CON + HN_2 \Rightarrow CHON + N_2$	10