

Supplementary Materials: Molecular Theory of Detonation Initiation: Insight from First Principles Modeling of the Decomposition Mechanisms of Organic Nitro Energetic Materials

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1. Modeling DADNE

In simulating an ideal DADNE crystal, we used $2 \times 2 \times 2$ Monkhorst-Pack k-point mesh and the kinetic energy cut-off was set to 520 eV. Atomic coordinates and lattice constants were allowed to simultaneously relax without any symmetry constraints. The convergence criterion for electronic steps was set to 10^{-5} eV, and the maximum force acting on any atom was set not to exceed 0.02 eV/Å. The calculated lattice constants, $a = 7.11$ Å, $b = 6.83$ Å $c = 11.558$ Å, were found to be in agreement with the experimental lattice constants $a = 6.941$ Å, $b = 6.569$ Å and $c = 11.56$ Å [116] within 4%.

Surface reactions were simulated in a slab model, in which the supercell with lattice consisted of the four-molecule-thick surface layer (appropriately cut out to create the (010) surface) on top of a 10 Å of vacuum. Surface supercell calculations we performed at the Gamma point only, with kinetic energy cut-off set to 520 eV. The convergence criteria for electronic and ionic steps were set to 10^{-5} eV and 0.03 Å/eV, respectively. Supercell has lattice parameters $a = 14.220$ Å, $b = 22.429$ Å and $c = 23.119$ Å and contains 32 molecules. Coordinates of unit cell and surface supercell are collected below.

2. Modeling TATB

In simulating an ideal TATB crystal, we used $2 \times 2 \times 3$ Monkhorst-Pack k-point mesh and the kinetic energy cut-off was set to 520 eV. Atomic coordinates and lattice constants were allowed to simultaneously relax without any symmetry constraints. The convergence criterion for electronic steps was set to 10^{-5} eV, and the maximum force acting on any atom was set not to exceed 0.02 eV/Å. The calculated lattice constants, $a = 9.207$ Å, $b = 9.232$ Å $c = 7.163$ Å, were found to be in agreement with the experimental lattice constants $a = 9.010$ Å, $b = 9.028$ Å and $c = 6.812$ Å [1] within 5%.

Surface reactions were simulated in a slab model, in which the supercell with lattice consisted of the four-molecule-thick surface layer (appropriately cut out to create the (001) surface) on top of a 10 Å of vacuum. Surface supercell calculations we performed at the Gamma point only, with kinetic energy cut-off set to 520 eV. The convergence criteria for electronic and ionic steps were set to 10^{-5} eV and 0.03 Å/eV, respectively. Supercell has lattice parameters $a = 18.433$ Å, $b = 15.971$ Å and $c = 20.176$ Å and contains 16 molecules. Coordinates of unit cell and surface supercell are collected below.

3. Coordinates

3.1. DADNE unit cell

1.0

7.1101876328689233	-0.0005603435561343	-0.0486170540142459	
-0.0005365011028712	6.8334751457089720	0.0000845972268726	
-0.2032549274931936	0.0001876858325154	11.5579975699804454	
H	C	N	O
16	8	16	16

Direct

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3.2. DADNE (010) surface

1.0

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0.0000000000000000 22.4291992188000009 0.0000000000000000
-0.5645396563000000 0.0000000000000000 23.1127067394999983

H C N O

128 64 128 128

Direct

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3.3. TATB unit cell

1.0

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H C N O

12 12 12 12

Direct

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