# Supplement information for Reaction mechanism and sensitivity enhancement of energetic materials doped with carbon nanotubes under electric fields by molecular dynamics simulations

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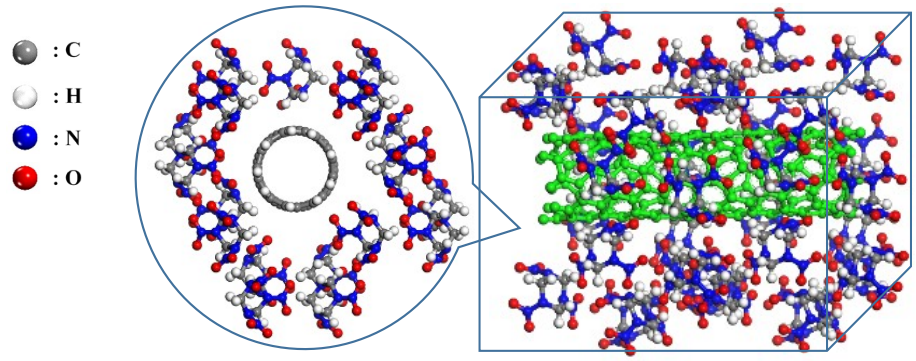
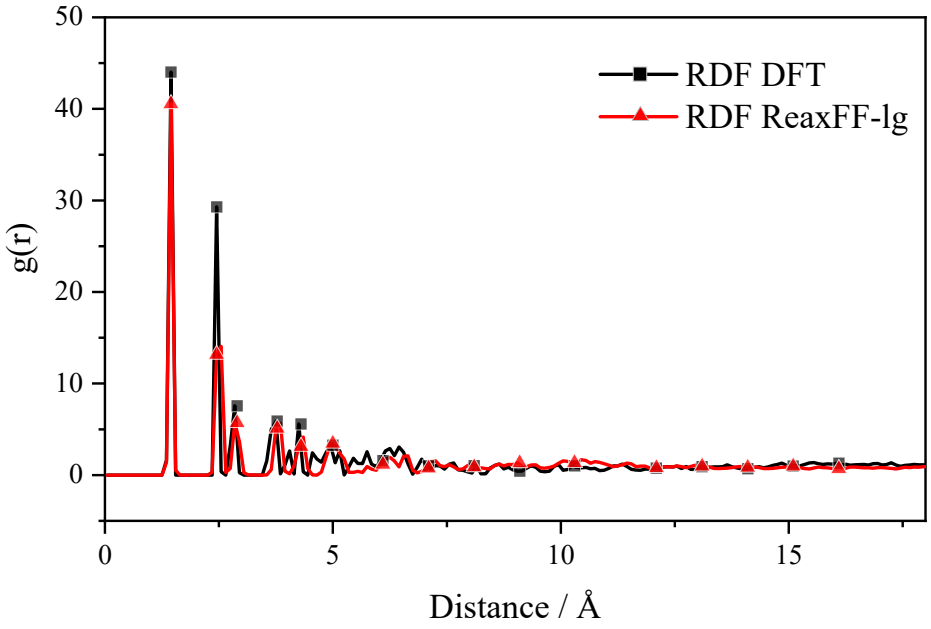
## Section 1

S.F.1 shows the QM model of RDX@CNT system. The QM calculations were based on density functional theory (DFT) using the DZVP-MOLOPT-SR-GTH level. S.F.2 shows the radial distribution function (RDF) of the RDX@CNT system predicted by MD/ReaxFF-lg and QM calculations.

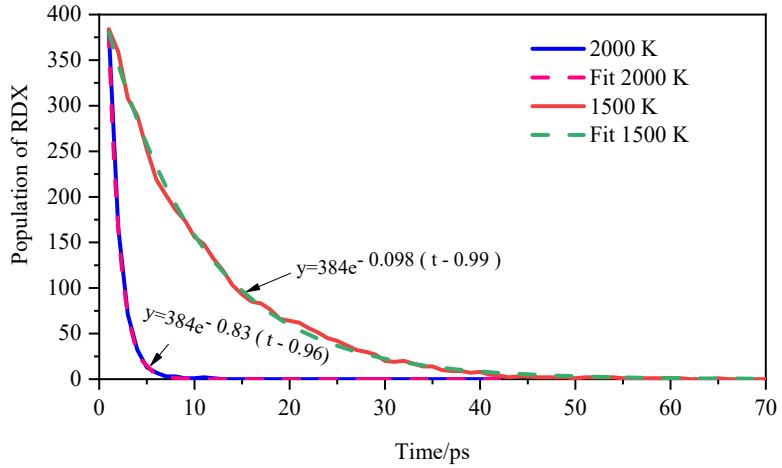



S.F.1 QM model of RDX@CNT system.

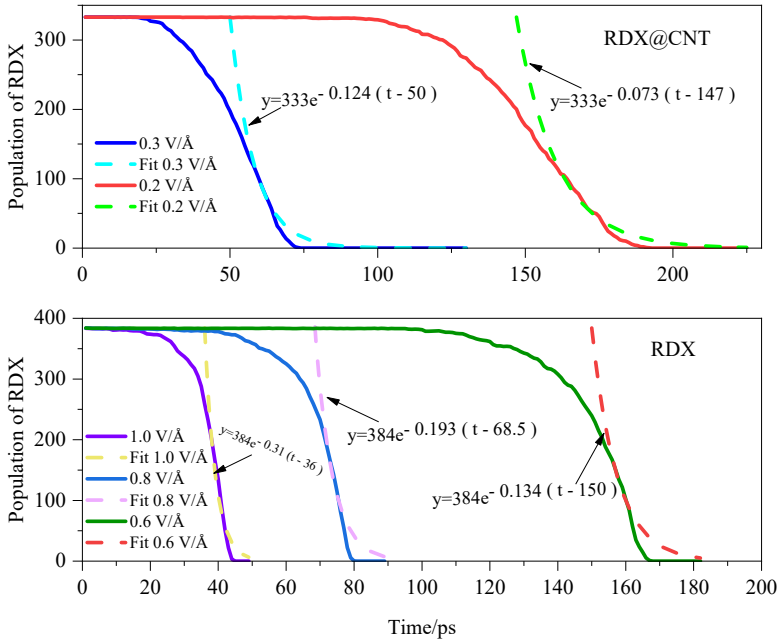



S.F.2 Radial distribution function

## Section 2




(a) Under high temperature

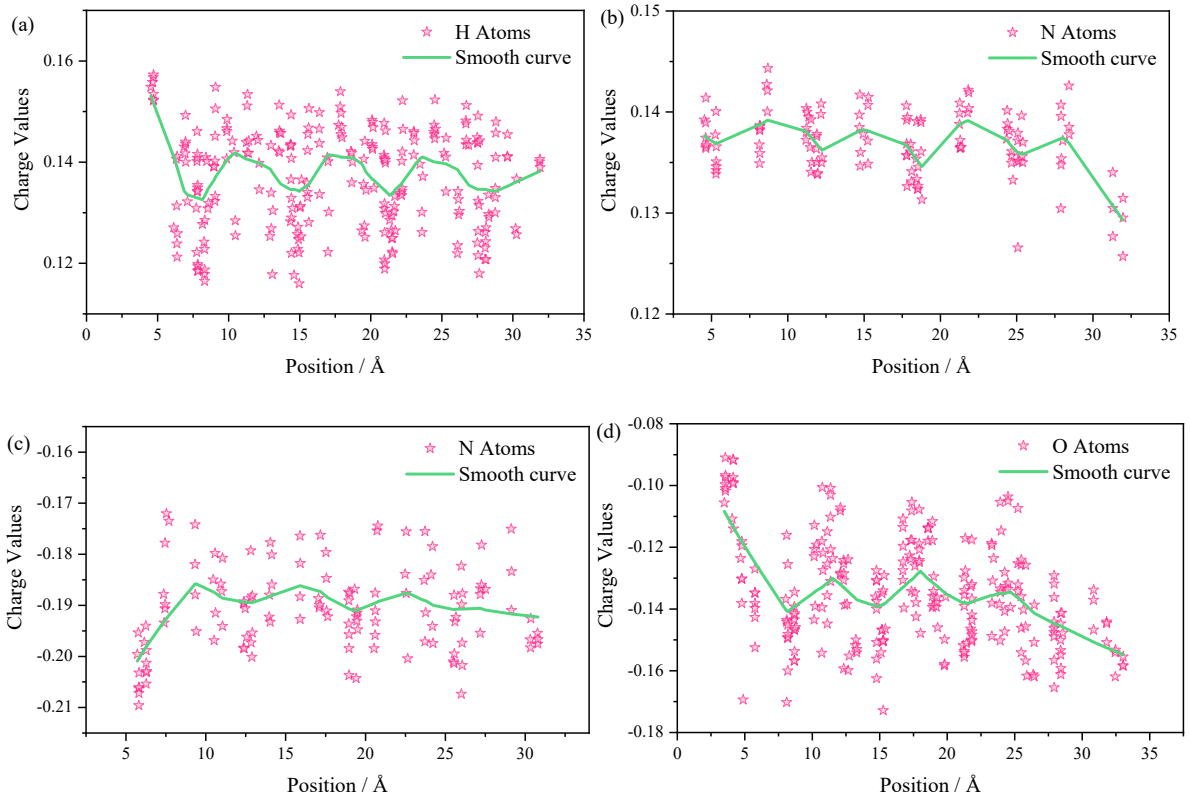



(b) Under the electric fields

S.F.3 The number evolution of RDX molecules of systems No.5, No.7, No.9, No.11, No.12, No.13 and No.14 and their fitting curves. (a) and (b) is the curves under different temperatures and under different electric fields.

## Section 3

S.F.4 illustrate the relationship between all charge values and the vertical coordinates for the RDX@CNT system, where (a)-(d) represent H atoms, N atoms in nitro groups, N atoms in the nitrogen heterocycle, and O atoms. We have smoothed the relationship curves and presented them in the figures. As can be seen from the figures, near the ends of the CNT molecule, i.e., around the vertical coordinate of 0, the charge values of RDX show significant deviations from the average, which is not evident in the computational results of the RDX system.




S.F.4 The relationship between all charge values and the vertical coordinates for the RDX@CNT system, where (a)-(d) represent H atoms, N atoms in nitro groups, N atoms in the nitrogen heterocycle, and O atoms.

# Section 4

## The code for LAMMPS

```
units           real
boundary        p p p
atom_style      charge
read_data       rdx.data
pair_style      reax/c NULL lgvdw yes
pair_coeff      * * ffield.reax.lg C H N O
neighbor        2 bin
neigh_modify    every 20 delay 0 check yes
variable        dt equal 0.1
variable        ef equal 0.5
timestep        $(v_dt)
reset_timestep  0
fix     1 all nve
fix     2 all qeq/reax 1 0.0 10.0 1e-6 reax/c
fix     3 all reax/c/bonds 2000 bonds.y
fix     in all efield 0 0 v_ef
thermo          50
thermo_modify   lost ignore flush yes
```

```
thermo_style        custom step time temp press vol density pe ke etotal cella cellb cellc cellalpha cellbeta cellgamma
dump                    4 all cfg 10000 laserhmx100.*.cfg mass type xs ys zs id
dump_modify         4 element C H N O
dump_modify         4 sort id
fix                   Specie all    reax/c/species 2 50 200 species.100 element C H N O
restart              100000 tmp*.restart
run                        10000000
```