

Supporting Information

Polymer Reinforced DNAN/RDX Energetic Composites:  
Interfacial Interactions and Mechanical Properties

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S-1. Energy expression used in COMPASS forcefield

The molecular forcefield is the key to the molecular dynamics simulations; in this research the Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) forcefield was used. The COMPASS forcefield was developed based on the CFF forcefield series, and has many cross-items in the energy expression to improve the accuracy of the calculations. The basic form of the energy expression used in the COMPASS forcefield is shown as follows:

$$\begin{aligned}
 E = & \sum_{bond} [K_{b2}(b-b_0)^2 + K_{b3}(b-b_0)^3 + K_{b4}(b-b_0)^4] + \\
 & \sum_{angle} [K_{a2}(\theta-\theta_0)^2 + K_{a3}(\theta-\theta_0)^3 + K_{a4}(\theta-\theta_0)^4] + \\
 & \sum_{dihedral} [K_{t1}(1-\cos\phi) + K_{t2}(1-\cos 2\phi) + K_{t3}(1-\cos 3\phi)] + \\
 & \sum_{OOPA} K_{\chi}(\chi-\chi_0)^2 + \sum_{bond/bond} K_{bb}(b-b_0)(b'-b'_0) + \\
 & \sum_{bond/angle} K_{ba}(b-b_0)(\theta-\theta_0) + \sum_{angle/angle} K_{aa}(\theta-\theta_0)(\theta'-\theta'_0) + \\
 & \sum_{bond/torsion} (b-b_0)(K_{bt1}\cos\phi + K_{bt2}\cos 2\phi + K_{bt3}\cos 3\phi) + \\
 & \sum_{angle/torsion} (\theta-\theta_0)(K_{at1}\cos\phi + K_{at2}\cos 2\phi + K_{at3}\cos 3\phi) + \\
 & \sum_{angle/torsion/angle} k(\theta-\theta_0)(\theta'-\theta'_0)(\phi-\phi_0) + \sum_{nonbond} \{\epsilon_{ij}[2(\frac{r_{ij}^0}{r_{ij}})^9 - 3(\frac{r_{ij}^0}{r_{ij}})^6] + \frac{q_i q_j}{r_{ij}}\}
 \end{aligned} \tag{S-1}$$

It may be seen that the non-bond interactions are included in the equation, and the van der Waals (vdW) interaction term used the form of Lennard-Jones (LJ) 9-6, for which the mixing rule is as shown in Equation S-2, thus the accurate vdW energy can be obtained from the calculations.

$$\left\{ \begin{aligned}
 r_{ij}^0 &= \left[ \frac{(r_i^0)^6 + (r_j^0)^6}{2} \right]^{1/6} \\
 \epsilon_{i,j} &= 2\sqrt{\epsilon_i \epsilon_j} \left[ \frac{(r_i^0)^3 (r_j^0)^3}{(r_i^0)^6 + (r_j^0)^6} \right]
 \end{aligned} \right. \tag{S-2}$$