Thermal Decomposition Mechanism of 1,3,5,7-Tetranitro-1,3,5,7-tetrazocane Accelerated by Nano-Aluminum Hydride (AlH₃): ReaxFF-Lg Molecular Dynamics Simulation

Ying Zhao, Zheng Mei, Feng-Qi Zhao, Si-Yu Xu, and Xue-Hai Ju*

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1. INTRODUCTION

Energetic materials (EMs) consisting of CHON elements are a class of significant substances containing a large amount of chemical energy. They can release huge amounts of energy after decomposition, which make them widely used in military and aerospace fields. Nevertheless, with the improvement of the requirement of comprehensive properties of EMs, conventional EMs cannot gradually meet the requirements of high energy density materials. As a result, a growing number of researchers are working to synthesize EMs with better properties. Alternatively, the addition of high active metal additives is an effective way to improve the properties of EMs. Research shows that EMs with high active metal additives have higher detonation and combustion properties. Commonly used high active metal additives include aluminum, magnesium, boron, and so forth. However, some studies have found that metal hydrides can replace metals as better additives to mix with EMs. Compared with metal power, metal hydrides possess high hydrogen storage capacity and higher combustion heat. Their decomposition can release large amounts of hydrogen, which allows them to release more energy and decline the average molecular weight of the gas in the combustion process. Common metal hydrides include MgH₂, CaH₂, AlH₃, and so forth. Among these metal hydrides, the application of AlH₃ is considered important for the development of EMs because of its high hydrogen storage capacity (10.1%). At present, AlH₃ has been successfully applied in solid propellants as an active additive. Compared with traditional propellants, the performance of propellants containing AlH₃ is greatly improved. For instance, Deluca et al. found that adding AlH₃ into propellants could increase the specific impulse. Moreover, in the application of active additive, the size of the particles also has an important effect on its properties. Some investigations have found that the reactivity of nano-Al powder obviously increases as the size decreases. Hence, it is important to study the influence of micron or even nanometer AlH₃ on explosives. However, because of the hazard of EMs and the instability of AlH₃, it is difficult to explore the mechanism of action of AlH₃ on explosives by experiments. Therefore, it is necessary to study the application of nano-AlH₃ in EMs theoretically. Reactive molecular dynamics (RMD) simulation is an effective method...
to investigate the reaction mechanism between nano-AlH₃ and EMs.

RMD can favorably describe the performance of large-scale systems and study the chemical reactions that may exist. It can simulate the free rupture and generation of chemical bonds between atoms, making it possible to analyze the chemical reaction process in the system. Besides, compared with quantum chemical methods, RMD has excellent simulation speed. RMD is primarily simulated using the ReaxFF force field. Furthermore, in order to describe the long-range interaction of atoms, ReaxFF-lg that uses a low-gradient (lg) model to correct long-range effects is developed based on ReaxFF. At present, ReaxFF-lg is being successfully applied to the study of large-scale systems containing CHONAl. However, there has been only limited studies on the effect of AlH₃ on the thermal decomposition of HMX.

In this paper, the ReaxFF-lg reaction force field with CHONAl parameters was used to perform the thermal decomposition of HMX and HMX/AlH₃ systems. The decomposition pathways, intermediates, products, evolution of AlH₃ clusters, and diffusion coefficients of each atom were analyzed through the C++ program developed by our group.

2. COMPUTATIONAL METHODS AND DETAILS

A ReaxFF-lg reactive force field containing CHONAl parameters was used to perform the RMD of HMX and HMX/AlH₃ systems. It has been proved that this force field is suitable for studying the thermal decomposition of high EM systems containing CHONAl. LAMMPS, the large-scale atomic molecular massively parallel simulator, was used to perform all simulations. ReaxFF-lg uses the following equation to determine the energy and then the force on each atom.

\[ E_{\text{system}} = E_{\text{bond}} + E_{\text{lp}} + E_{\text{over}} + E_{\text{under}} + E_{\text{angle}} + E_{\text{double}} + E_{\text{triple}} + E_{\text{tors}} + E_{\text{conj}} + E_{\text{Hbond}} + E_{\text{vdWaals}} + E_{\text{Coulomb}} \]

where \( E_{\text{bond}} \) is the bond energy, \( E_{\text{lp}} \) is the lone pair energy, \( E_{\text{over}} \) and \( E_{\text{under}} \) are over- and under-coordination corrections, respectively, \( E_{\text{angle}} \) is the bond angle energy, \( E_{\text{double}} \) and \( E_{\text{triple}} \) are double- and triple-bond corrections; \( E_{\text{tors}} \) is the dihedral angle energy; \( E_{\text{conj}} \) is the conjugation energy; \( E_{\text{Hbond}} \) is the hydrogen bond energy; \( E_{\text{vdWaals}} \) is the van der Waals energy; and \( E_{\text{Coulomb}} \) is the electrostatic energy.

In this work, HMX supercell was derived from the extended original cell of \( \beta \)-HMX (P2\( _1 \)\( n \)). The orthogonal HMX(001) supercell was built through Materials Studio 7.0 tools. The spherical AlH₃ nanoparticle with a diameter of 4.0 nm was obtained by cutting the supercell obtained from the extended \( \alpha \)-AlH₃ crystal. Moreover, in practical applications, in order to maintain reactivity, the nano-AlH₃ particles are usually covered with an oxide layer. However, the diameter of the nano-AlH₃ model constructed in this work is only 4 nm, which is far smaller than the size of the nano-AlH₃ particles in practice (about 100 nm). Therefore, in order to maintain the reactivity of aluminum hydride, only core–shell aluminum hydride particles coated with 0.1 nm oxide layer were established. First, MS tool was used to cut aluminum oxide balls with a diameter of 4.8 nm. A self-made C++ program was used to embed the 4 nm aluminum hydride into aluminum oxide with internal vacuum to form aluminum hydride nanoparticles coated with 0.1 nm aluminum oxide on the surface. The constructed core–shell aluminum hydride particles were fully relaxed under the NVT ensemble of 30 ps. The result is the core–shell aluminum hydride particles shown in Figure 1. In order to embed aluminum hydride particles in the center of the box, the orthogonal HMX(001) supercell was built, and then the AlH₃ and AlH₃O particles were embedded into the HMX(001) supercell to build HMX/AlH₃ and HMX/AlH₃O composite systems. The thickness of the vacuum layer between both particles and HMX molecules is 0.2 nm. Figure 1 presents the model of the HMX/AlH₃ composite. Molecular dynamics simulation was performed to relax the HMX, HMX/AlH₃, and HMX/AlH₃O particles after embedding are shown in yellow and green, respectively.

Figure 1. Construction process of the composite model. C, H, O, and N atoms are shown in gray, white, red, and blue, respectively. AlH₃ and AlH₃O particles after embedding are shown in yellow and green, respectively.
HMX/AlH₃O systems in the isobaric–isothermal (NPT) ensemble up to 20 ps (300 K). The properties before and after the relaxation of the two systems are listed in Table 1.

Table 1. Properties of HMX and HMX/AlH₃ Systems

| Model         | Composition          | Mass Fraction of AlH₃ (%) | Initial Density (g/cm³) | Relaxed Density (g/cm³) |
|---------------|----------------------|---------------------------|------------------------|-------------------------|
| HMX           | 420 HMX              | 1.96                      | 2.04                   |
| HMX/AlH₃      | 411 HMX + Al₁₀H₂₀₂₀   | 19.74                     | 1.50                   | 1.94                    |
| HMX/AlH₃O     | 455 HMX + Al₁₀H₂₀₂₀O₃ | 23.35                     | 1.65                   | 1.90                    |

Here in, aluminum and hydrogen in the aluminum hydride particle accounted for 19.74 and 23.35% of HMX/AlH₃ and HMX/AlH₃O, respectively. In practical application, the additive proportion of aluminum hydride can reach 10–30% in weight. After that, a canonical ensemble (NVT) was used to simulate the thermal decomposition of both the models. In the NVT simulation process, the initial temperature was set as 300 K and then increased to 3500 K within 100 ps, followed by 100 ps constant temperature simulation at 3500 K. The main reason is that 3500 K is more in line with the temperature after the explosive explosion. On the other hand, the decomposition of the system is more complete at 3500 K. The time step was 0.1 fs. A Nose–Hoover barostat and a thermostat were used to control the pressure and temperature during the NPT and NVT simulations. The charge distribution method is the QEq method, and the tolerance value is set as 1 × 10⁻⁶. The coupling parameter is 10. Moreover, 30 ps NVE was used to simulate the ignition reasonably for HMX and HMX/AlH₃ in highly confined spaces almost without mass and heat transfer. In the species analysis, the bond-length cutoff is 1.2 times the standard single bond length. When the distance between atoms is larger than the standard bond length, the bond is considered ruptured.

3. RESULTS AND DISCUSSION

3.1. Applicability of the Calculation Method. Radial distribution function can provide information about the probability of finding an atom in a spherical shell at a distance \( r \) from an arbitrary atom. According to the distribution of atomic probability at \( r \), we can understand the interaction distance between atomic pairs in the crystal, that is, the length of the chemical bond between the two atoms. Hence, the 3 × 3 × 3 of AlH₃, 2 × 2 × 2 of α-Al₂O₃, 3 × 3 × 3 of AlC₃, 3 × 3 × 3 of AlN, 3 × 3 × 3 of Al, and 3 × 3 × 3 of HMX supercells were established to relax under a 30 ps NPT ensemble; here in, all crystal protocols come from the crystallography open database. The final 5 ps structure of the supercell was used to analyze the radial distribution function between atomic pairs. In the radial distribution function, the first peak tends to represent the nearest pair of atoms, that is, the length of the bond in the crystal. Figure 2 presents the radial distribution function between atomic pairs in the HMX crystal. In the HMX supercell, the first peak of \( r_{\text{C-H}} \) is 1.075–1.175 Å, and the experimental of the HMX crystal shows that the C–H bond length range is 1.093–1.0981 Å. The first peak of \( r_{\text{C-N}} \) is 1.465–1.525 Å, and the C–N bond length in the experimental is 1.436–1.480 Å. The first peak of \( r_{\text{N,O}} \) is 1.275–1.315 Å, and the N–O bond length in the experimental is 1.252–1.260 Å. The first peak of \( r_{\text{O,N}} \) is 1.485–1.525 Å, and the N–N bond length in the experimental is 1.374–1.525 Å. To sum up, it can be observed that there is little difference between the experimental value and the calculated value. The results show that the method is suitable for HMX system simulation.

Figure 2 presents the calculated radial distribution function between atomic pairs of AlH₃, α-Al₂O₃, AlC₃, AlN, and Al crystals. In α-Al₂O₃, the first peak between O and Al occurs at 1.815–2.095 Å. Based on the experimental crystal structure of α-Al₂O₃, the minimum and maximum values of O–Al bond length are 1.843 and 1.982 Å, respectively. The first peak of \( r_{\text{O,Al}} \) is 1.815–2.025 Å. In AlH₃, the first peak of \( r_{\text{H,Al}} \) is 1.825–1.915 Å, and the minimum and maximum values of the C–Al bond length in AlC₃ crystal are 1.769 and 1.784 Å. In AlC₃, the first peak of \( r_{\text{C,Al}} \) occurs at 1.875–2.225 Å, and the minimum and maximum values of the C–Al bond length in the AlC₃ crystal are 1.898 and 2.223 Å. In AlN, the first peak of \( r_{\text{N,Al}} \) is 1.895–2.025 Å, and the minimum and maximum values of the C–Al bond length in the AlC₃ crystal are 1.893 and 1.894 Å. In Al, the largest peak of \( r_{\text{Al,Al}} \) is 2.855 Å, and the length of the Al–Al bond in the Al crystal is 2.852 Å. Hence, the calculated value is close to the experimental value. This further confirms the accuracy of the method used in the simulation in describing the interaction with Al atoms.

3.2. Adsorption of HMX on the Surface of AlH₃ Crystals in NPT Simulation. In the relaxation process of HMX/AlH₃ and HMX/AlH₃O systems, both AlH₃ particle surfaces strongly attract HMX molecules, causing some HMX molecules to absorb on the AlH₃ particle surface. Figure 4 shows that the AlH₃ particles of HMX were adsorbed on the surface. Figure 5 shows the variation of bond numbers of AlH₃–Al, AlH₃–O, AlH₃–Al, AlN, and Al crystals.
position trigger bond in HMX is not ruptured. Figure 4 shows the reduction proportion in the HMX quantity and released energy during NPT simulation. It can be seen from Figure 6 that the adsorption reaction between HMX and aluminum hydride particles results in the decomposition of HMX, and the adsorption process was a spontaneous exothermic reaction. This spontaneous reaction is caused by the strong attraction of Al to the O atoms in HMX. Compared with HMX/AlH₃, the increasing number of O–Al and N–Al bonds and the decreasing number of N–O bonds in the HMX/AlH₃O system are smaller. This indicates that the presence of oxide layer, to a certain extent, inhibits the reactivity between aluminum hydride particles and HMX in the adsorption stage. Nevertheless, the HMX molecule reacts with both the particles depending on the attraction of Al to oxygen. This can be judged from the large increase of O–Al bonds between the two systems during the adsorption phase. In addition, the adsorption reaction stops after 15 ps because of the stable passivation layer formed by the adsorption of HMX on the surface of aluminum hydride. These results indicate that HMX/AlH₃ composites can exist stably under certain conditions.

3.3. Heating and Adiabatic Simulations. Figures 7 and 8 present the evolution of HMX molecules and the corresponding potential energy (PE) from 300 to 3500 K within the NVT ensemble. In the PE calculation, all PEs are referenced by the PE values of the relaxed system and divided by the number of HMX molecules in the system. It can be observed that the decomposition of pure HMX begins at about 1100 K. Hereafter, the HMX decomposition rate accelerates rapidly with the increase of temperature. Nevertheless, in the HMX/AlH₃ system, the attraction of AlH₃ can lead to the decomposition of some HMX molecules in the relaxation process, and HMX/AlH₃ starts to decompose after 5 ps heating. The variation of PE shows that the decomposition of HMX/AlH₃ is an exothermic reaction without energy barrier. However, there is an energy barrier of 133.57 kcal/mol for the decomposition of pure HMX system. Moreover, it can be noted that HMX/AlH₃ shows much higher reaction heat than HMX from Figure 7.

In order to explore the decomposition path of these three systems, the evolution of the number of bonds is calculated and illustrated in Figure 9. In terms of the tendency of bonds to decrease in Figure 9 (HMX), the scission of N–N bonds and C–H bond are the main decomposition pathways of pure HMX. It is consistent with other experimental and theoretical studies.²⁰–²¹ However, the decomposition pathway in HMX/AlH₃ and HMX/AlH₃O is different from that in pure HMX. It can be noted that the rate of decrease of N–O bonds is significantly higher than that of other bonds from Figure 9 (HMX/AlH₃, HMX/AlH₃O). The results demonstrated that the scission of N–O bonds is the dominating pathway of HMX in HMX/AlH₃ and HMX/AlH₃O. Moreover, in HMX/AlH₃ and HMX/AlH₃O systems, the decreasing rate of C–N bonds becomes relatively quick after the heating up of the system, indicating that AlH₃ particles cause the C–N bond to break easily. Nevertheless, in the same simulation time, the reduction of N–O and C–N bonds in the HMX/AlH₃O system is much smaller than that in the HMX/AlH₃ system. The results show that the oxide layer inhibited the reactivity of aluminum hydride.
The NVE simulations can describe the ignition reasonably for EMs in highly confined spaces with less mass and heat transfer. Hence, the adiabatic processes of HMX and HMX/AlH₃ systems are simulated by the NVE ensemble. The evolution is preceded by preheating of 2 ps at 1500 K within the NVT ensemble. It is worthwhile to point out that the 1500 K preheating ignites the EM system. Figure 10 presents the evolution of HMX molecules, PE, and temperature within the NVE ensemble. These profiles show clearly that the decomposition rate determines the PE release rate and the temperature increase rate of the adiabatic system. The rate of overall decomposition, energy release, and temperature increase of AlH₃/HMX is much larger than those of the HMX system. Moreover, Figure 8 clearly exhibits the remarkably low rate of energy release and temperature rise within the 5–15 ps. This is consistent with the fact that HMX decomposition in NVT simulations requires a large number of barriers.

3.4. Evolution of Al-Containing Clusters. The evolution of the components of Al-containing clusters was analyzed to study the role of Al in the decomposition process of HMX/AlH₃. Figure S1 shows the evolution curve of the X–Al bond of HMX/AlH₃/O system. Figure 11 reveals the evolution of X–

Figure 11. Evolution of X–Al (X presents C, H, O, or N) bond of Al-containing clusters in the NVT simulation.

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Figure 12 presents the configurations of Al-containing clusters with HMX molecules in the NVT simulation. Herein, OVITO program is used to analyze the variation of Al-containing clusters, and the cutoff distance of the cluster is set to 3.5 Å. As can be seen from Figure 12, in the process of reaction between HMX molecules and AlH₃ particles, CHO atoms in the HMX molecule gradually enter the inside of AlH₃ particles to oxidize Al atoms with the increase of temperature, while the Al in AlH₃ spreads outward. This result causes holes to form inside the AlH₃ particles. Figure 13 presents the variation of the number of Al-containing clusters. It can be observed that the number of Al-containing clusters increases dramatically in 0–30 ps because the structure of AlH₃ is
destroyed as temperatures rise and oxygen atoms penetrate. After that, Al-containing clusters are gradually oxidized to form alumina. Despite the increase of temperature, it is difficult to make a significant change in the number of Al-containing clusters within 30−80 ps. However, the replacement reaction mentioned above and the high temperature (>2220 K) after 60 ps cause a sharp increase in the number of Al clusters. The substitution of C and the high temperature destroy the structure of alumina, causing the aluminum clusters to melt, disperse, and agglomerate (Figure 12; 100, 110, and 120 ps). When the temperature reaches 3500 K, the C−Al clusters fuse at high temperature (Figure 10; 150 ps). As a result, the number of Al-containing clusters decline rapidly. The reaction of C and N−Al clusters makes the number of Al-containing clusters increase slowly until the Al-containing clusters dominated by C−Al bond are formed.

3.5. Stable Products and Major Intermediates. Figure 14 illustrates the evolution of stable products in HMX and HMX/AlH₃ systems. Figure S2 shows the evolution of stable gaseous products of the HMX/AlH₃O system. It can be noted that the evolution of gaseous products is basically consistent in HMX/AlH₃ and HMX/AlH₃O systems. Hence, only HMX and HMX/AlH₃ systems are discussed. Consistent with previous experimental and theoretical studies, the final stable products of HMX system thermal decomposition are N₂, H₂O, and CO₂, of which N₂ is the largest amount, while CO₂ is the least amount. These gas products start to form after 50 ps (at 1200 K), and accumulate rapidly to a peak. Comparatively, the amount of stable products in HMX/AlH₃ is different from that in the HMX system. In addition to the formation of Al-containing clusters, it is observed that H₂O is the most abundant product in HMX/AlH₃ and its amount is much larger than that in the HMX system. However, the amount of N₂ is reduced, and no CO₂ is produced. Moreover, in the HMX/AlH₃ system, N₂ and H₂O can be produced rapidly at low temperatures. As temperatures rise, these gases are produced at a high rate before 100 ps; after that, they achieve the maximum (150 ps) yields in a relatively slow rate. The productions of H₂O and N₂ after 100 ps are related to the decrease of N−Al and O−Al clusters discussed previously in 3.1 (Figure 10). The formation of H₂O indicates that H₂ also reacts with O−Al clusters. Consequently, the peaks of product numbers are delayed in the HMX/AlH₃ system in comparison with pure HMX. Meanwhile, the results also show that the combustion time in HMX/AlH₃ has been extended.

These stable gas productions have important influences on the performance of the propellant. Although the amounts of N₂ and CO₂ in the HMX/AlH₃ system are reduced, the amount of H₂O increases significantly, and the total gas yield of HMX/AlH₃ is larger than that of the HMX system. Furthermore, HMX/AlH₃ system reduces emission of carbon dioxide; it is favorable for the protection of the environment. Figure S3 presents the evolution of pressures under the NVT ensemble. It can be noted that the rate of pressure increase and the final stability value in the HMX/AlH₃ system are larger than those in the HMX system.

Figure 15 presents the evolutions of the main intermediates during the decomposition process of HMX and HMX/AlH₃.

Figure 12. Configurations of Al-containing clusters with HMX molecules in the NVT simulation. C, H, O, N, and Al atoms are shown in gray, white, red, blue, and pink, respectively.

Figure 13. Variation of the number of Al-containing clusters in the NVT simulation. Cutoff distance of the neighbor cluster model is 3.5 Å.

Figure 14. Evolution of products in NVT simulation.

Figure 15. Evolution of intermediates in the decomposition process of HMX and HMX/AlH₃.
that these intermediates are mainly composed of O-containing free radicals and unstable products containing O atoms in pure HMX, indicating that O atom plays an important role in the process of HMX decomposition. In HMX/AlH₃ and HMX/Al₂H₆O, H₂ as the most important intermediate is produced first due to the decomposition of AlH₃ at low temperature. Although there are O-containing intermediates in the decomposition of HMX/AlH₃ and HMX/Al₂H₆O, their amounts are significantly reduced. Among these O-containing intermediates, OH is the most abundant and the first to be produced in HMX/AlH₃ and HMX/Al₂H₆O, which is different from that in HMX. The results indicate that the decomposition pathway of HMX in HMX/AlH₃ and HMX/Al₂H₆O systems is different from that of pure HMX. Considering the evolution of Al–X discussed above, it can be known that the strong attraction of AlH₃ particles to O atoms causes HMX to decompose prematurely. Meanwhile, the binding effect of Al on CNO atoms makes these atoms difficult to interact with each other to form O-containing intermediates, and the active H₂ reacts easily with O to form OH, causing OH to become the most intermediate in the decomposition process of HMX/AlH₃ and HMX/Al₂H₆O.

3.6. Diffusion Analysis. The diffusion analysis can quantitatively describe the atomic interactions in the decomposition process. Hence, the diffusion coefficients of all atoms in these two systems were calculated. Diffusion coefficient is calculated by Einstein’s diffusion equation, which is mean square displacement (MSD) divided by time and then divided by 6 (three-dimensional diffusion). The MSD is the average of displacement of each type of atoms, as \( \langle r(t)^2 \rangle = r(0)^2 + 6Dt \). \( r(0) \) is the initial coordination of an atom. In this work, the MSD is computed every 1 picosecond to calculate the current diffusion coefficient. Figure 16 presents the average diffusion coefficient of atoms in HMX and HNM/AlH₃ systems. The magnitude of diffusion coefficient is related to the relative atomic mass. Therefore, the diffusion coefficient of H atom is the largest in both systems. Nevertheless, although O has a larger relative atomic mass than C and N, the diffusion coefficients of C and N are less than that of O. The phenomenon indicates that there are other factors influencing the diffusion of atoms in the decomposition process of HMX. In combination with the intermediates in HMX decomposition discussed earlier, O atoms are involved in more intense chemical reactions. Meanwhile, it can be observed that the diffusions of C, N, and O in HMX are larger than those in HMX/AlH₃. This is because some of the CNO atoms are attracted to Al, making them difficult to spread. However, the diffusion of H in HMX/AlH₃ is larger than that in HMX. This is because H₂ produced by decomposition of AlH₃ participates in violent chemical reactions. However, C is easily deposited on aluminum particles, and its diffusion coefficient decreases most obviously. The result is consistent with the phenomenon that the final Al-containing cluster is dominated by C–Al.

4. CONCLUSIONS

The ReaxFF-lg reactive field was used to simulate the thermal decomposition process of HMX and aluminum hydride nanocomposite system. The simulation results show that aluminum hydride changes the initial decomposition mechanism of the HMX molecule. HMX was first adsorbed on the surface of hydrogenated aluminum particles and then decomposed by a new way of N–O bond and C–N bond. The strong attraction of aluminum to oxygen and the medium attraction to nitrogen are the main reasons for the change of HMX initial decomposition mechanism. The increase of O–Al and N–Al bonds in the evolution of aluminum-containing clusters confirms this view. During the oxidation of aluminum hydride particles, a large number of oxygen atoms and a small number of N atoms permeate into the interior of aluminum hydride particles. The aluminum atoms of aluminum hydride spread out. The internal structure of aluminum hydride is destroyed, forming hydrogen accumulation cavity. As the temperature increases, hydrogen breaks through the outer oxide layer and participates in the intermediate reaction. Because of the ability of H₂ to compete for oxygen atoms, the H₂O yield of HMX/AlH₃ system increases and the CO₂ yield decreases. The adiabatic simulation indicates that energy release and temperature increase of AlH₃/HMX are much larger than those of the HMX system.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.0c02968.

Evolution of X–Al (X presents C, H, O, or N) bond of Al-containing clusters in HMX/AlH₃O; evolution of products of HMX/AlH₃O in NVT simulation; evolution of system pressure during NVT simulation; and evolution of intermediates in the decomposition process of HMX/AlH₃O (PDF)

AUTHOR INFORMATION

Corresponding Author

Xue-Hai Ju — Key Laboratory of Soft Chemistry and Functional Materials of MOE, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China; orcid.org/0000-0002-9668-3066; Email: xhju@njjust.edu.cn

Authors

Ying Zhao — Key Laboratory of Soft Chemistry and Functional Materials of MOE, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China
Zheng Mei — Key Laboratory of Soft Chemistry and Functional Materials of MOE, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China
Feng-Qi Zhao — Science and Technology on Combustion and Explosion Laboratory, Xian Modern Chemistry Research Institute, Xian 710065, P. R. China
Si-Yu Xu — Science and Technology on Combustion and Explosion Laboratory, Xian Modern Chemistry Research Institute, Xian 710065, P. R. China

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.0c02968

Notes
The authors declare no competing financial interest.

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