HMX/NMP Cocrystal Explosive: First-Principles Calculations

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Abstract

The band structure, total density of states and atomic orbit projected density of states analysis were performed to investigate HMX/NMP cocrystal by using the first-principles calculations. Results show that the HMX/NMP cocrystal is equipped with a direct band gap and the interactions between HMX and NMP molecules are rather weak. The O orbits hybridize with H orbits and the parts of charge transform from H to O atoms by analyzing the DOS. The HMX/NMP cocrystal possesses three types of intermolecular interactions between HMX and NMP, these interactions and the arrangement of two molecules in the structure are the main reasons for the low sensitivity of the cocrystal. The C-H...O type hydrogen bond is the key role in forming the structure, and the strength of the hydrogen bond interaction for C-H...O-N is higher than that of C-H...O-C.

1. Introduction

Energetic materials usually refer to organic compounds containing energy-containing groups (such as nitro, amino and azide groups) in molecules, which release significant quantities of energy in an instant when there is a chemical reaction [1–4]. Energetic materials have a wide range of applications, for example, their chemical energy can be used to do work for missile launch and can be used as gas generators [5]. Explosives, propellants and pyrotechnics are common energetic materials, which are widely used in civil and military fields [6–8]. A great deal of research has been done on energetic materials, such as 2,4,6-trinitrotoluene (TNT), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) [1, 9]. Among these typical energetic materials, HMX is one of the most commonly used traditional explosives in propellants and explosives, it was first discovered as a by-product of synthesis of RDX in 1930 [8] and its molecular structure is similar to RDX, with the characteristics of high energy density, high melting point and high explosive performance [1, 8–10]. However, ideal energetic materials should have the advantages of good detonation performance as well as the low thermal and impact sensitivity [1, 11]. It is difficult to meet the requirements of insensitive high density energetic materials (IHDEMs) [12, 13] for HMX due to its moderate sensitivity [8, 11], so the effective methods to reduce the sensitivity of HMX without significant energy reduction has aroused extensive attention in the academic circle [14, 15].

Cocrystallization, which is the result of intermolecular interactions between two or more neutral molecules such as hydrogen bonds, π -stacking, and van der Waals forces [16, 17]. Studies show that the sensitivity of HMX with inert molecules cocrystal is usually lower than that of pure HMX [8, 18] and it is a promising method to solve this problem [16]. N-methyl-2-pyrrolidone (NMP) with a carbonyl group, it is a unique functional group and it is solvent molecule [4, 18, 19]. It is reported that the cocrystallization of HMX and NMP is helpful in reducing the sensitivity of the explosive [18, 20]. In 1985, Haller and Rheingold et al. [21] prepared the HMX/NMP cocrystal by cooling crystallization for the first time and obtained the lattice parameters of the structure. In 2013, Lin and Zhu et al. [22] prepared the HMX/NMP cocrystal by solution evaporation method and investigated host-guest interactions of the structure by using the first-principles calculations. But as far as we know, the calculations of electronic properties for the HMX/NMP

cocrystal by Lin et al. are inaccurate, as can be seen from the band structure and state density diagrams (the parts above the Fermi level are missing). In addition, for cocrystal, intermolecular interactions are the key to the formation of cocrystal structure and are mainly contributed by the intermolecular hydrogen bond interactions [16]. It is of great significance to analyze the intermolecular interactions which may reduce the sensitivity in cocrystal [11, 23]. Therefore, combined with the above situation, it is very necessary to re-analyze the electronic properties and intermolecular interactions of the HMX/NMP cocrystal.

In our study, we calculated the band structures and the density of states using the first principles, and focused on analyzing its electronic properties and the possible intermolecular hydrogen bond interactions. The research results of this paper as the complement published in 2013 by Lin et al. [22] and we hope to provide some reference and guidance for the design of HMX/NMP cocrystal in the future.

2. Computational Methods

In this work, the first principles calculation of HMX/NMP cocrystal were performed using the CASTEP (Cambridge Sequential Total Energy Package) code [24] based on density functional theory (DFT) [25, 26] with GGA [27] in the scheme of Perdew-Burke-Ernzerhof (PBE). The cutoff energy of 380.0 eV for the plane-wave was used and the K-points in the Brillouin zone was set to $1 \times 1 \times 1$ throughout all calculations. The electronic configurations of the ions used for the calculation are $2s^2 2p^2$ of C, $1s^1$ of H, $2s^2 2p^4$ of O, $2s^2 2p^3$ of N. In the calculation, we used the experimental data [21] as the structural parameters for calculation and optimized the atomic positions. The atom coordinates for HMX/NMP cocrystal are shown in Table 1, the values in parentheses correspond to the experimental data.

Table 1
The atom coordinates of HMX/NMP cocrystal.

Atom	x	y	z
C1	0.52581 (0.52880)	0.08519 (0.08190)	0.20758 (0.20700)
C2	0.44166 (0.44000)	-0.09638 (-0.09750)	0.21260 (0.21410)
C3	0.33333 (0.33333)	-0.20064 (-0.19828)	0.41447 (0.41667)
C4	0.48111 (0.45830)	-0.00582 (-0.02660)	0.41856 (0.42780)
C5	0.25194 (0.21140)	-0.29607 (-0.022340)	0.39989 (0.40060)
C6	0.33333 (0.33333)	-0.02918 (-0.05138)	0.41667 (0.41667)
C7	0.27004 (0.21500)	-0.11211 (-0.15320)	0.44417 (0.40500)
N1	0.35910 (0.36540)	-0.01534 (-0.01110)	0.19921 (0.19080)
N2	0.44371 (0.44620)	-0.00832 (-0.00960)	0.20665 (0.20210)
N3	0.53699 (0.52550)	0.13598 (0.12820)	0.24664 (0.24460)
N4	0.54067 (0.53460)	0.22123 (0.21610)	0.24504 (0.24130)
N5	0.30431 (0.30500)	-0.17189 (-0.13180)	0.45290 (0.41460)
O1	0.29407 (0.29510)	-0.09249 (-0.08640)	0.18855 (0.18960)
O2	0.35440 (0.37260)	0.05602 (0.06470)	0.20281 (0.18310)
O3	0.54689 (0.53860)	0.26098 (0.25650)	0.27910 (0.27390)
O4	0.53860 (0.53790)	0.25234 (0.24520)	0.20968 (0.20520)
O5	0.33333 (0.33333)	0.04347 (0.01692)	0.41667 (0.41667)

3. Results And Discussion

3.1 Crystal structures

The selected bond lengths in HMX/NMP cocrystal along with the corresponding experimental data [20] are shown in Table 2. It can be seen that the bond lengths compare well with experimental values which indicates that our results agree well with the experimental values. The calculated structure of the HMX/NMP cocrystal model viewed along the x axis is shown in Fig. 1. As seen from Fig. 1, HMX and NMP molecules are arranged in a staggered manner in the structure, which makes the whole crystal structure compact and contributes to the stability of the crystal structure [28–31]. The HMX/NMP cocrystal is a trigonal structure with the space group $R\bar{3}c$ and the lattice parameters are $a = b = 16.607 \text{ \AA}$ and $c = 31.506 \text{ \AA}$ [21], the molecular formula is $C_9H_{17}N_9O_9$. Figure 2 shows more detailed structural information of the HMX/NMP cocrystal. The arrangement of HMX and NMP molecules viewed along the

z axis is shown in Fig. 2 (a) [21], it can be seen that these two molecules are in a disordered arrangement in the cocrystal. Figure 2 (b) and (c) show the HMX molecule and NMP molecule with atom numbering. For HMX molecule ($C_4H_8N_8O_8$), there are three clearly defined structural motifs in HMX cocrystals, namely, chair – chair/layered, chair – chair/pocket, and chair/layered [8]. As can be seen in Fig. 2 (b), the HMX molecule shows the chair-chair ring conformation [19, 20] in HMX/NMP cocrystal, and there are four nitro groups on the same side of the C_4N_4 ring [32].

Table 2
Selected bond lengths along with experimental data in HMX/NMP cocrystal.

Bond	Length (Å)	Bond	Length (Å)
C1-N2	1.468 (1.444)	N4-O3	1.237 (1.221)
C1-N3	1.450 (1.441)	N4-O4	1.236 (1.237)
C2-N2	1.458 (1.464)	N1-O2	1.231 (1.226)
C2-N3	1.447 (1.455)	N3-N4	1.387 (1.373)
N1-O1	1.240 (1.222)	N1-N2	1.370 (1.370)

3.2 Electronic properties

The calculated energy band structures along the high symmetry direction of the Brillouin zone is shown in Fig. 3, the vertical dashed line at 0 eV is Fermi level. It can be seen that the valence band minimum (VBM) and the conduction band maximum (CBM) are both located at G point, this indicates that the HMX/NMP cocrystal shows direct bandgap behavior, the value of direct bandgap is 0.958 eV. In addition, the valence bands and conduction bands of band structures are quite flat along different symmetry directions in the Brillouin zone, which suggests that it is limited for overlap between orbitals on neighboring molecule, and the interaction between HMX and NMP molecules is rather weak in the cocrystal [33, 34].

In order to get more information about the electronic properties of the HMX/NMP cocrystal, we calculated the DOS (density of states) as shown in Fig. 4. Combining with TDOS (total density of states) and PDOS (partial density of states), the main characteristics of DOS can be summarized as follows. (1) These peaks are sharp and localized from PDOS, this indicates that the interactions in the cocrystal are weak, these peaks are associated with previous flat band structure (Fig. 3). (2) The density of states near Fermi level originates predominantly from N-2p, C-2s, C-2p and H-1s states, the density of states of C-2s and O-2p orbits are approximately zero at Fermi level. (3) At the bottom of conduction band region, the peaks are dominated by N-2p and O-2p orbits. At the top of valence band region, the peaks are mainly contributed by N-2p and H-1s orbits. (4) The density of states in the energy range of - 15 eV to - 14 eV originates predominantly from N-2p and C-2s states, their peaks occur around - 14.5 eV, this means that strong hybridization between the N-2p and C-2s states. Meanwhile, the PDOS shows that there is a hybridization between N-2p and O-2p at -2 eV. (5) The conduction bands around 3 eV are mainly composed of the hybridization interactions between C-2p and H-1s. (6) There is a hybridization between

O-2p and H-1s states in the energy range of -3 eV to -1 eV and 2 eV to 3 eV. This indicates that there is interaction between the O atom and H atom. Meanwhile, it is worth noting that the density of states from O-2p is mainly located below Fermi energy (-3 eV to -1 eV) which indicates that charge partially transferred from the weak H atoms to the strong O atoms [21, 33].

3.3 Intermolecular interactions

Intermolecular interactions are the primary drive forces for the formation of cocrystal and they contribute to the stability of the crystal structure [35, 36]. The hydrogen bonding is considered as one of the intermolecular interactions in numerous studies [37–41] and they are usually expressed in terms of X-H...Y [42–44]. For HMX/NMP cocrystal, the intermolecular hydrogen bond interactions between HMX molecule and NMP molecule are the main forces for the formation of HMX/NMP cocrystal, especially the hydrogen bond interaction between nitro group in HMX and neighboring hydrogen [35, 36]. In most of the examples of hydrogen bonds, the distance between H and Y atoms is less than the sum of their van der Waals radii [37, 38, 45]. Therefore, it can be preliminarily inferred the existence of hydrogen bond between O and H atoms when their distance is less than the sum of their van der Waals [45] for HMX/NMP cocrystal [8, 33, 38, 46]. In this study, we used 1.20 Å and 1.52 Å as the van der Waals radii of H and O [45], respectively.

Based on this method, we find the possible existence of hydrogen bonds between O5 and H16, O5 and H17, O6 and H19, O6 and H25, O7 and H19, O8 and H24, O9 and H20, O9 and H24, O9 and H26, O10 and H21, O11 and H21. The possible hydrogen bonds between HMX and NMP moleculars are shown in Fig. 5. In the Fig. 5 (a), the hydrogen bonds are indicated by the dotted lines, the HMX and NMP moleculars connected to each other by these possible hydrogen bonds. The H atoms of the methylene groups in HMX or the H atoms in the NMP molecular serve as proton donors, and the O atoms of the nitro groups in HMX or the O atoms in the NMP molecular serve as proton acceptors. We can see that there are three different intermolecular interactions between HMX and NMP moleculars in HMX/NMP cocrystal from Fig. 5 (b). These three types of intermolecular interactions play important roles in stabilizing cocrystal, combined with other weak interactions such as C...N interactions, finally form the structure. The distances and angles of possible hydrogen bonds found in cocrystal have been listed in Table 3, the labeled atoms are shown in Fig. 5 (b). In these possible hydrogen bonds, the shortest contact is C11H24...O8 with 2.091 Å and the longest one is C8H19...O6 with 2.611 Å. In addition, their bond angles are above 110° except the C10H20...O9 and C11H26...O9. It is reported in previous literature [37, 38] that the hydrogen bond angle should preferably be above 110° , the bond angles of these bonds are basically consistent with this conclusion. HMX and NMP molecules are alternately arranged in the cocrystal structure and connected by these hydrogen bonds, which increase the stability of the structure and safety of the cocrystal explosive. And this is one of the reasons for the decreased sensitivity of this cocrystal explosives [28–31, 47–49].

Table 3
The possible intermolecular hydrogen bonds in the HMX/NMP
cocrystal.

X-H...Y	X-H (Å)	H...Y (Å)	X...Y (Å)	∠X-H...Y (°)
C1-H16...O5	1.094	2.224	2.948	121.564
C2-H17...O5	1.088	2.282	2.866	130.947
C8-H19...O7	2.128	2.471	4.368	143.408
C8-H19...O6	2.128	2.611	4.690	163.417
C9-H25...O6	3.800	2.499	4.700	134.436
C10-H20...O9	1.081	2.356	2.716	89.134
C10-H21...O10	1.091	2.449	3.336	137.529
C10-H21...O11	1.091	2.379	3.314	142.673
C11-H24...O8	2.125	2.091	3.494	111.969
C11-H24...O9	2.125	2.350	4.195	139.179
C11-H26...O9	3.800	2.216	4.195	84.026

The electronic overlap in PDOS is generally interpreted as one of the evidence of the interaction for non-bond atoms [32, 33, 46]. In order to further study these interactions, we present the PDOS of the correlative O and H atoms (O5, O6, O7, O8, O9, O10, O11, H16, H17, H19, H20, H21, H24, H25, H26) in the HMX/NMP cocrystal as shown in Fig. 6. From Fig. 6 (a), it can be observed that resonance is found between O5 and H16 from - 7 eV to - 5 eV. The resonance is also found between O5 and H17 from - 6 eV to - 5 eV, especially their peaks appear at the same level with - 5.5 eV. This indicates that hydrogen bond interactions occur between O5 and H16, O5 and H17. Similarly, in the Fig. 6 (b), there are hydrogen bond interactions between O6 and H119 states in the energy range of - 10 eV to - 9 eV. And in the energy range of - 4 eV to - 2 eV, there are hydrogen bond interactions between O6 and H25 states. As Fig. 6 (c) – (e) show, the hydrogen bond interactions also occur between O9 and H20, O9 and H26, O7 and H19, O8 and H24. This is basically consistent with the previous results obtained by the distance method to determine the existence of hydrogen bond interactions. In addition, these hydrogen bond interactions can be divided into two types: C-H...O-C and C-H...O-N hydrogen bonds. The hydrogen bond interactions between O5-2p in NMP molecules and H-1s states (H16 and H17) belong to C-H...O-C hydrogen bonds, the other hydrogen bond interactions between other O-2p (O6, O7, O8 and O9) states in HMX molecules and H-1s states belong to C-H...O-N hydrogen bonds. It can be seen from the Fig. 6 that the hydrogen bonds in HMX/NMP crystal mainly comes from the C-H...O-N hydrogen bonds. Therefore, the strength of the hydrogen bond interactions for C-H...O-N is higher than C-H...O-C hydrogen bonds in the HMX/NMP cocrystal explosive.

4. Conclusions

In summary, based on the density functional theory, we have studied the electronic properties and intermolecular interactions by analyzing its band structure and the density of states. The main results and conclusions were summarized as follows in this study: 1. There is a direct band gap in the HMX/NMP cocrystal. 2. The interaction between HMX and NMP molecules is rather weak due to its bands being quite flat and its peaks from PDOS are localized. 3. There are hybridization interactions between N-2p and O-2p states, O-2p and H-1s states, N-2p and C-2s states, C-2p and H-1s. 4. There is interaction between the O atom and H atom, the parts of charge transform from H to O atoms. 5. Three types of intermolecular interactions play important roles in stabilizing the HMX/NMP cocrystal, and the C-H...O hydrogen bond interaction is the key role. 6. The arrangement of HMX and NMP molecules in the structure and the hydrogen bonds between them are the main reasons for the decrease of the sensitivity of the cocrystal. 7. The strength of the hydrogen bond interactions for C-H...O-N is higher than that of C-H...O-C hydrogen bond interactions.

Declarations

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Conflicts of interest/Competing interests

All authors declare that we have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this manuscript.

Availability of data and material

The data sets supporting the results of this work are included within the article, the other datasets generated during the current study are available from the corresponding author on reasonable request.

Code availability

Not applicable

Authors' contributions

Yi-Hua Du: Writing - original draft, Formal analysis, Investigation, Methodology, Software

Fu-Sheng Liu: Data curation, Methodology, Writing - review & editing

Qi-Jun Liu: Conceptualization, Project administration, Resources, Supervision, Writing - review & editing

Bin Tang: Methodology, Software, Writing - review & editing

Mi Zhong: Data curation, Writing - review & editing, Visualization

Ming-Jian Zhang: Investigation, Methodology, Writing - review & editing

Ethics approval

Not applicable

Consent to participate

Not applicable

Consent for publication

Not applicable

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Figures

Figure 1

The crystal structures of HMX/NMP cocrystal viewed along the x axis.

Figure 2

(a) The arrangement of HMX and NMP molecules viewed along the z axis; (b) the molecular structure of HMX; (c) the molecular structure of NMP.

Figure 3

Band structure of HMX/NMP cocrystal.

Figure 4

DOS of HMX/NMP cocrystal.

Figure 5

(a) The possible hydrogen bonds between HMX molecule and NMP molecule found in cocrystal; (b) three intermolecular interactions between HMX and NMP in cocrystal (the hydrogen bonds are indicated by the dotted lines).

Figure 6

The PDOS of the O and H atoms in the HMX/NMP cocrystal: (a) O5 and H16, O5 and H17, (b) O6 and H19, O6 and H25, (c) O9 and H20, O9 and H24, O9 and H26 (d) O7 and H19, O8 and H24, (e) O10 and H21, O11 and H21.