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ORIGINAL PAPER

Ab *initio* molecular dynamics simulation on the formation process of He@C_{60} synthesized by explosion

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Abstract The applications of endohedral non-metallic fullerenes are limited by their low production rate. Recently, an explosive method developed in our group shows promise to prepare He@C_{60} at fairly high yield, but the mechanism of He inserting into C_{60} cage at explosive conditions was not clear. Here, ab initio molecular dynamics analysis has been used to simulate the collision between C_{60} molecules at high-temperature and high-pressure induced by explosion. The results show that defects formed on the fullerene cage by collidsion can effectively decrease the reaction barrier for the insertion of He into C_{60}, and the self-healing capability of the defects was also observed.

Keywords Ab initio molecular dynamics · Collision · Explosion · He@C_{60}

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Introduction

Endohedral fullerenes have received great attention because of their application in many fields such as pharmacy [1], quantum computing [2], materials science [3–5], etc. The inner space of fullerene is suitable to entrap small atoms or clusters [6], especially metallic atoms [7]. It is difficult to synthesize noble atom encapsulated fullerenes, because the reaction force between the cage and the atoms is too small to stabilize the complex [6, 8]. So far, some endohedral non-metallic fullerenes have been synthesized by different methods but with low yields of 0.4 % to 1 % [8–15].

The ability to perform a "molecular surgery", which involves the open and close of the fullerene, may provide a new approach toward the encapsulation of certain atoms during the open process. A successful example is that Kei Kurotobi et al. has entrapped H_2O and H_2 into C_{60} by molecular surgical approach [12, 15]. On the other hand, ion bombardment techniquesion can also break the C_{60} cage to facilitate the insertion of He, Ne and other atoms [16, 17]. However, neither of the above two methods could closely meet the requirements of both high yield and high efficiency. Obviously, the main reason of the low yield for noble atoms comes from the high reaction barrier to penetrate the C_{60} cage. Ohtsuki et al. suggested that it needs 130 eV for Xe and 80 eV for Kr to insert into C_{60} through the six-membered ring [18]. In the case of He insertion into C_{60}, generally the energy needed for penetration is around 8.7 to 12 eV [19–21]. For instance, tight-binding approach by Granot indicated that the kinetic energy of He penetrating C_{60} need at least 12 eV [21]. For Patchkovskii's calculations 8.7 eV barrier is obtained by semiempirical, ab initio and density functional [19], but the related energy barrier may be expected to be larger than 10 eV by the biased transition path sampling approach from molecular-dynamics simulation [20]. Recently, Peng et al. have successfully prepared He@C_{60} at the yield of 4 % through an explosive method

(EM) [22]. This method possesses the merits of timely efficient and cost-effective, but the explosive process and mechanism are rather complex, which are extremely difficult to be modeled with a comprehensive and systematic solution. Moreover, the obscure reaction mechanism makes it rather difficult to adjust the experimental parameters, which forbids further improvement of the reaction efficiency.

To solve the bottle-neck problem, ab initio molecular dynamics (AIMD) simulation has been carried out in this paper to investigate the collision of C_{60} at atomic level and the formation process of He@C_{60} synthesized by EM. We suggest that if the defects on C_{60} cage are formed by losing carbon atoms, the traveling of He atoms in and out of the C_{60} cage becomes viable with a much lower barrier of 3.0 eV. Further studies show that the collisions between C_{60} molecules driven by explosion plays a crucial role in facilitating the formation of those defect. Besides, after He inserts into C_{60}, the defects can self-heal at the explosive environments.

Experimental and theoretical details

In the previous experiments based on EM [22], C_{60} powder (150 mg, >99.9 %) and explosive of HMX (cyclic-$[CH_2N\text{-}NO_2]_4$, 1 g) was initially put into the experiment apparatus at ca. 0.6 atm He. After detonation, the nearly instantaneous explosion produced a shock wave that accelerated He and C_{60} molecules collision in the experiment apparatus because of their extremely high speeds. Meanwhile, the temperature reached up to 2000–5000 K and pressure raised to 10–30 GPa in $10^{-6}\sim10^{-7}$ s [23]. These shock velocities came from HMX or RDX are typically from 4 to 9×10^3 m s^{-1} by theoretical calculation [24–26]. To experimentally study explosion shock wave, a method of small scale gap test was improved to guarantee the steady propagation of shock wave, a Mn-Cu manometer was used to measure the detonation pressure (23.5–28.8 GPa), and the range of detonation velocity was 2 to 5×10^3 m s^{-1}.

AIMD simulation within the framework of density functional theory (DFT) implemented in the CP2K/Quickstep package was carried out to stimulate the collision of fullerenes for the He@C_{60} synthesized [27–29]. CP2K/Quickstep package is based on the hybrid Gaussian and plane wave method. The Gaussian functions which consisted of a double-ζ plus polarization (DZP) basis set were employed to optimize the molecules structure. The energy cutoff for the real space grid used to represent the density was 320 Ry. Perdew, Burke and Ernzerhof (PBE) exchange-correlation functions [30] were used to simulate the collision between two C_{60} molecules. For some cases, the exchange correction of Becke and the correlation function of Lee, Yang and Parr (BLYP), local density approximation (LDA) and PBE plus van der Waals dispersion corrections (PBE-vdw) [31] were also used to calculate the interaction energy between He and C_{60}. In our AIMD simulation, we carried out with the initial speeds of the molecules in the range of 2.32×10^3 and 3.28×10^3 m s^{-1}, as mentioned above. We determined the energy of the potential barrier for He inserts into C_{60} (and C_{58}) using the climbing image nudged elastic band (NEB) method [32, 33]. In the NEB method, a set of images (N=12) is uniformly distributed along the reaction path connecting the initial and final states optimized in our simulation. To ensure the continuity of the reaction path, the images are coupled with elastic forces, and each intermediate state is fully relaxed in the hyperspace perpendicular to the reaction coordinate [33].

Results and discussion

Theoretical analysis: interaction energy of HeC_{60}

We investigated the interaction of He with C_{60}. To determine the preferred site of He on C_{60} surface, we first calculated the interaction energy of HeC_{60} by placing the He atom on the pentagonal, hexagonal sites, carbon-carbon bond and a carbon atom, wherein the atom moved inward speeding up in the shock waves. It was an important step in the formation process of He@C_{60}. Here, the interaction energy of them is defined as follows:

$$E_{com} = E_{HeC60} - (E_{C60} + E_{He}), \quad (1)$$

where E_{com} is the interaction energy compared with various exchange-correlation functions, E_{HeC60} is the total energy of fullerenes complex, E_{C60} and E_{He} are the total energy of a free molecule He and C_{60}, respectively. We calculate the formation energies of He and C_{60} through PBE, PBE-vdw, BLYP, BLYP-vdw and PADE exchange-correlation functional, the He and C_{60} cage was obtained using the optimizations of the atomic geometries.

The results show that the interaction energy between He and C_{60} is about $0.01\sim-0.04$ eV with our calculation, where the interaction energy is found for a distance of 3.40 Å of the He from the C_{60} surface, which is in agreement with earlier calculations [34]. The results show a weak attractive interaction between them, it means there are many possibilities for the geometry of He and C_{60} complex because they nearly remain isolated from each other. We consider the geometry of He and C_{60} as this corresponds to the experiment apparatus, a question that need to be answered is as follows: how does He get into C_{60} in the shock wave, through a hexagonal (C6) or pentagonal (C5) of the perfect C_{60}?

Energy barrier of the formation process of He@C_{60}

There are two kinds of rings on C_{60} cage, C5 and C6. Obviously, C6 has larger space for He to insert than C5 and other sites of C_{60}, thus we mainly consider how He inserts into C_{60} through C6.

Figure 1 shows that the reaction experiences for He insert into C_{60} through the center of a of C6 perpendicularly, which was explored with NEB method. The initial and final states correspond to He staying outside and inside C_{60} as shown in Fig. 1a and c, respectively. The transition state is that one He atom inlaid within the C6, as a result of the cage deformed considerably, which can be seen in Fig. 1b. The lengths of C-C bonds are greatly increased by 0.1 and 0.2 Å relative to perfect C6, and the computed barrier for He inserting is 9.7 eV. The C6 restore its previous state after He goes into C_{60} as we can see in Fig. 1c.

In this case, the He penetrates into the cage through the center of the C6 with difficulty, since the atom radius of He is 0.31 Å, the hole of a C6 is not large enough for He to be in and out of the C_{60} cage freely. Thus the main energy barrier for He inserting into C_{60} is used to enlarge the origin C6.

Such a large barrier greatly hampers the inserting process of He into C_{60} and this should be the main reason that the production yield is rather low in most of the experimental studies [16, 17]. That is, it does not provide a direct penetration of a He through the center of a C6 occurs with suitably high kinetic energy in the explosion.

As mentioned above, both He and C_{60} will be accelerated by the shock wave in the experimental conditions, thus they have great chance to collide together in a very short time, and the original C_{60} may generate all kinds of defects in such processes because of the collision. In order to check whether the defect of C_{60} can lower the reaction barrier and enhance the production yield, the reaction barrier of He inserting into C_{60} with defect was also studied. Divacancy may be generated either by collision of C_{60} or high-pressure and high temperature [35]. For such calculations, the typical defect and divacancy are used to study the reaction barrier.

As we know, C_{60} is generally known to undergo consecutive C2 eliminations in what used to be called the Rice shrink-wrap mechanism [36]. That means C_{58}, C2 eliminations on C_{60}, contains two kinds of ring, one is a 7-membered ring (C7) and the other is an 8-member ring (C8). C8 has a relative larger space than C6, thus it may be easier for He to pass through C8 than C6. To more accurately simulate process of He insert into C_{58} through C7 and C8, the C_{60} expel C2 unit and undergo cage shrinking was simulated in AIMD, The unimolecular dissociation channels for C_{60} is shown in Eq. (2):

$$C_{60} \rightarrow C_{58} + C2. \quad (2)$$

The structure of C_{58} contains C7 when C_{60} expel C2 unit in the adjacent hexagon, or contains C8 when C_{60} expel C2 unite in the adjacent pentagon (see Fig. 2b and c).

As shown in Fig. 2a and d, in the prefect C_{60}, the energy calculations showed that the He penetrates through the center of the C6 with a large energy of 9.75 eV. and the barriers for He inserting into C_{58} are 5.36 and 3.00 eV for C7 and C8 (Fig. 2b, c and d), respectively. Compared with the energy 9.75 eV for He inserting into perfect fullerene, the divacancy on the fullerene can effectively lower the reaction barrier. That is to say, He@C_{60} can be more easily fabricated from the fullerene with defect than the perfect.

C_{60} collisions caused by shock wave

To further reveal the formation mechanism of He@C_{60} at explosive condition, we simulate C_{60} collision in the shock wave condition. The contact point and position of the initial structures of two C_{60} did not describes in the model of collision. C_{60} is based on one-dimension face-to-face collision under shock wave condition as mentioned by Jakowski et al. [37], namely, kinetic energy (or the velocities of the molecules) will be a major factor in deciding the final structures. It is suggest that the simulation provides a realistic way to depict the highly complex molecules collision in the experiment apparatus.

Under the explosive condition, a very high speed was imposed on C_{60} by shock wave of HMX. C_{60} molecules from opposite directions have a great chance to collide with each other at very high speed. In the process of collision,

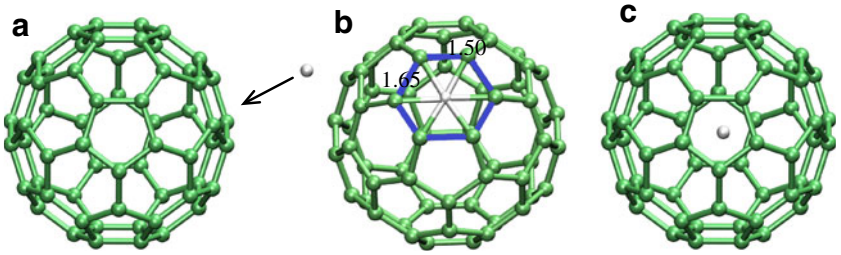

Fig. 1 The reaction path for He inserting into C_{60} through C6 by NEB method. **a** the initial state of He staying outside of C_{60} and the arrow is the path of He to be inserted into C_{60} through a C6, **b** the transition state of He atom inlaid in a C6 and the bond length of the C6 increased from 1.41 to 1.50 and 1.45 to 1.65 Å, **c** the final state of He@C_{60}

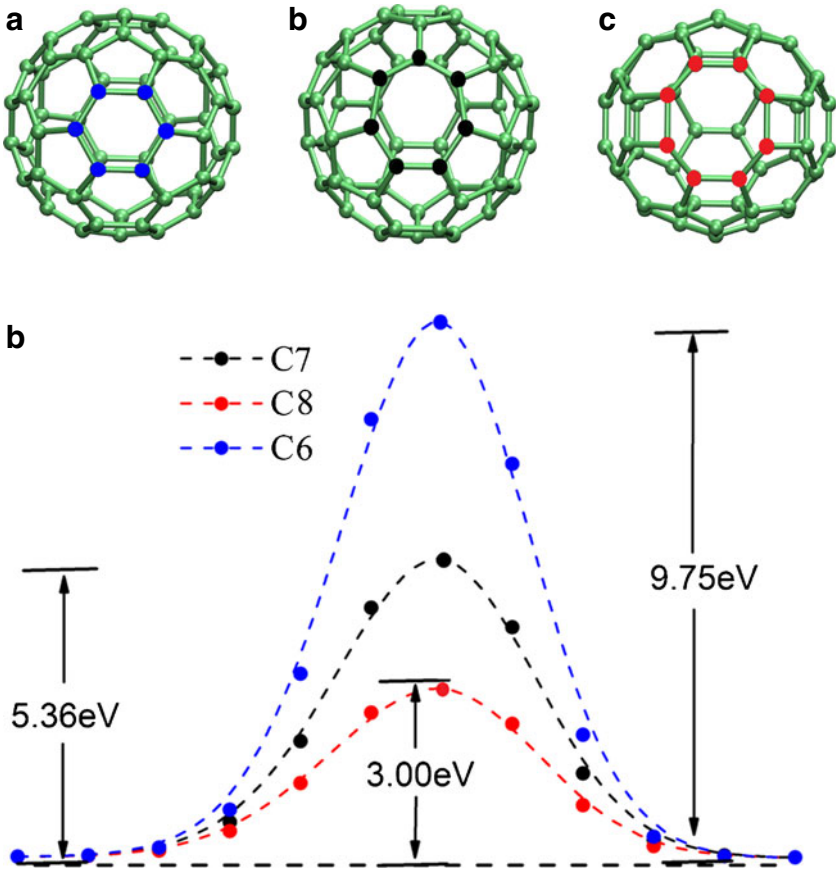

Fig. 2 The energy barrier for He inserting the C_{60} and C_{58}. **a**, **b**, **c** show the atomic structure of C6 on C_{60}, and C7, C8 on C_{58} respectively. **d** shows the energy barriers for the He insert into the fullerenes through C6, C7 and C8

defects may be formed on some C_{60} cages. In order to understand the detailed information of C_{60} collision, several AIMD simulations were carried out with different initial speeds in the range of 2.32×10^3 to 3.28×10^3 m s^{-1}. The AIMD results show that when the initial speed of C_{60} is lower than 2.59×10^3 m s^{-1}, the C_{60} will bounce quickly, and no reaction occurs after this process. When the initial speeds of C_{60} are higher than 3.00×10^3 m s^{-1}, the two C_{60}s collide to form defects on their cages.

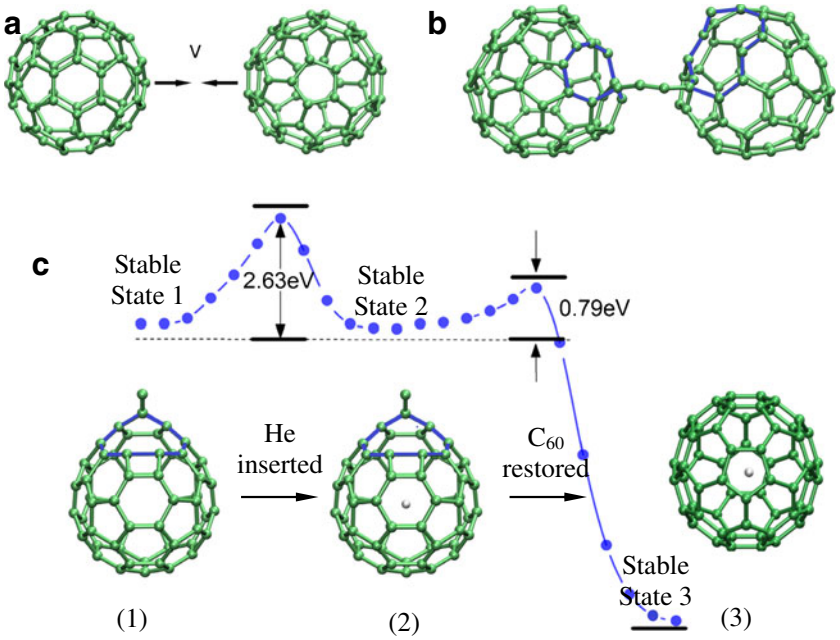

Fig. 3 The structural evolution of an orifice in the collision with a velocities(V) and encapsulation of He to open-cage C_{60}. **a** Initial structures of two C_{60} molecules, **b** a C9 and C11 orifice of an open-cage C_{60} dimer was formed, **c** the minimum energy reaction barrier path of He inserting into C_{60} cage through a C9 orifice and restoration of the orifice for synthesis of He@C_{60}. (1), (2), (3) show the stable states in the path for He insert into the C_{60}, through C9

AIMD simulation with the collision kinetic energy of 40 eV (3.28×10^3 m s^{-1}) shows the collision-induced reactive case in Fig. 3. Figure 3a shows the initial structures of two C_{60} molecules face-to-face collision under shock wave condition. In our simulation, a pentagonal bond is first broken, and then a series of C-C bonds are broken and reorganization occurred, which lead to one of C_{60} opening a window. The orifice becomes larger because two pentagonal bonds are broken. A C11 of C_{60} dimer was formed in such process as shown in Fig. 3b. Although the C11 of the dimer is a transition state, considering window mechanisms, the transition structures for the passage of He through C11 windows needs to be verified. As a matter of fact, the dimer was easily separated by the collision of other fullerenes and molecule (e.g., C, NO, NO_2 from explosion) in explosive atmosphere. The binding energy of the dimer separation is 6.8 eV as an independent molecule.

Similarly, in order to realize the C11 windows of an independent molecule, the molecular geometries were fully optimized. Ultimately, both of the C_{60}s were evolution of an orifice with C9 (shown in Fig. 3c).

AIMD simulations show that C_{60} will form defects during the collision process in the explosive conditions. Such results agree with Brink's experiment on endohedral fullerene collision which also suggests a large hole formation on fullerene cage [38] and shown by chemical method [11].

Figure 3c shows the stable states for the passage of He through C9 have been located and fully characterized at the PBE level, the He insertion with 2.63 eV shows that the energy barrier is obviously lower than the perfect C_{60}. Compared with the atom structure with the perfect C_{60}, only the C-C bonds of C6 are extended, thus the small structure change should be the main reason for the lower energy barrier for the He inserting into C_{60} during the collision. Saunders et al. have studied that the He release from the C_{60} with an energy barrier of 0.99~3.5 eV through an opened window in a fullerene on experimental work [11, 39], which would be in agreement with our calculation in such explosive conditions. Consequently, a defect formed by carbon atoms loss from the C_{60} can lower the reaction barrier and improve the productive yield for He@C_{60}. In addition, the orifice of C9 can easily restore to the perfect one with a barrier of 0.79 eV as shown in Fig. 3c.

As we can see, the shock wave from the explosion can not make the He insert into the perfect C_{60} directly, it may be limited by the kinetic energy of the He. Instead of this, opening an orifice on the C_{60} by collisions between molecules under the explosions was the main reasion to get the high yields of He@C_{60}. It suggests that the formation process of He@C_{60} can be separated into three key steps. The first step is C-C bonds breaking and the defect forming through collision process of C_{60} molecules, and this step is the most important step. The second step is He inserting into C_{60} through the defect and the last step is the self-restoration of the cage. The whole reaction mechanism mimics the self-healing method.

Conclusions

AIMD simulations have been carried out to explore at the atomic level the formation process of He@C_{60} synthesized by EM. Although He@C_{60} can be generated through a direct inserting process, the rate is very low considering that the reaction barrier is rather high (about 10 eV). Our results show that the He@C_{60} can easily be formed by means of inserting He into C_{60} through opening an orifice on the cage. The main reason is that the EM can generate defected C_{60} in a very short time through collisions between C_{60} molecules, and He can be quickly inserted into the defected C_{60}. After such processes, the defected cages can be restored by other C atoms to form He@C_{60} in the atmosphere. Our results suggested that He inserting into C_{60} by EM is by a "window" mechanism. Such result paves an important way in understanding the formation process of He@C_{60} at explosive atmosphere.

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To experimentally study explosion shock wave, a method of small scale gap test was improved to guarantee the steady propagation of shock wave, a Mn-Cu manometer was used to measure the detonation pressure (23.5–28.8 GPa), and the range of detonation velocity was 2 to 5×103 m s^{-1}. It was found that there is a close relation between explosion shock wave of explosive quality and the yields of $He@C_{60}$