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Depressing thermal conductivity of fullerene by caging rare gas

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HIGHLIGHTS

- We have investigated the thermal conductivity of C_{60} and its derivatives caged with rare gas by using the nonequilibrium molecular dynamics method.
- We found that embedding C_{60} with different rare gas atoms has a significant impact on its thermal conductivity.
- A phenomenon was observed that the thermal conductivity of C_{60} can be depressed by adding rare gas in it.
- We build a one-dimensional C_{60} chain and find that its thermal conductivity can be influenced by embedding rare gas in each C_{60}.

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ABSTRACT

We have investigated the thermal conductivity of C_{60} and its derivatives caged with rare gas by using the nonequilibrium molecular dynamics method. It is reported that embedding C_{60} with different rare gas atoms has a significant impact on its thermal conductivity. We analyze the phenomenon through the phonon spectra of rare gas atom and the C–C bonds length of C_{60}. When the number of atoms inside the C_{60} increases, the phonon spectra band width of rare gas expands and the length of C–C bonds becomes longer, which contributes to the depression of the thermal conductivity of C_{60}. The method is applied to control the thermal conductivity of C_{60} chains, which maybe a kind of potential materials in thermal circuits. Our results also provide a controllable method for the thermal management in nanoscale materials.

1. Introduction

Due to various underlying applications of fullerene (C_{60}), more and more scientific attention has been given to their exceptional and unique physical and chemical properties since its discovery in 1985. In the latest field of materials science, fullerene and its derivatives have become widely used as electron-acceptors because of their remarkable electron acceptor ability, which are applied to organic electronics and sensing [1] as well as artificial photosynthetic systems [2,3]. Plenty of applications about fullerene have been reported in the area of science and technology, especially in the field of photovoltaic devices [4]. In virtue of its high permeability through biological barriers [5], antioxidant properties and the ability to entrap metals and small molecules [6], fullerene is proposed in biomedical research which can provide valuable information on molecular interactions. Owing to its potential usage both in non-linear optics [7,8], and single-molecule transistors [9,10] along with its tunable electronic properties resulting in superconducting or semiconducting behavior [10–12], fullerene has drawn considerable attention in respective fields.

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In low-dimensional system, thermal conductivity is quite a vigorous research field [13], resulting in the development of many thermal devices [14], such as thermal resistance and thermal transistor [15], thermal memory [16] and thermal rectifier [17,18], which have been reported in both theory and experiment in the past few decades. Numerous attention has been focused on the study of the thermal conductivity of graphene and carbon nanotubes. Although there are substantial studies in biomedical and chemical science of C_{60}, the research on its thermal conductivity and what can change or how to change the thermal conductivity of C_{60} remains limited.

It was reported that the thermal conductivity of C_{60} as well as C_{70} is about 0.5–2 W/mK at room temperature [19–21], which indicates that C_{60} can be used as good thermal insulating materials. More and more studies suggest that C_{60} caged with metal or gas atoms will show interesting physical and chemical properties [22,23]. Thus, it is expected that C_{60} caged with gas atoms will perform an astonishing thermal property.

In this paper, the thermal conductivity of C_{60} and the ways of changing it are studied by using nonequilibrium molecular dynamics method. The changing rules of thermal conductivity of C_{60} are also investigated, which are closely related to the average temperature of C_{60}. A phenomenon was observed that the thermal conductivity of C_{60} can be depressed by adding rare gas in it. This phenomenon can be interpreted by the changes of the phonon spectra and C–C bonds length after adding rare gas. Furthermore, we build a one-dimensional C_{60} chain and find that its thermal conductivity can be influenced by embedding rare gas in each C_{60}. The obtained results are of significance when attempting to change the thermal conductivity of single C_{60} in a multiply C_{60} system.

2. Model

In our molecular dynamics (MD) simulation model, the thermal conductivity of a certain material structure is studied by designing heat transferred across the material. This is realized by connecting each end of the structure to a hot and a cold heat bath respectively. Here we apply the Nose–Hoover thermostat as the heat bath. In this paper, we focus on two structures: single C_{60} molecular and C_{60} chain. Each of the C_{60} may cage one or more rare gas atoms in it. Fig. 1 shows the single C_{60} molecule centered with one rare gas atom. In order to reduce the influence of boundary effect, the tested C_{60} is connected to two C_{60}. Here we use rare gas atom as the core simply for their stable chemical properties.

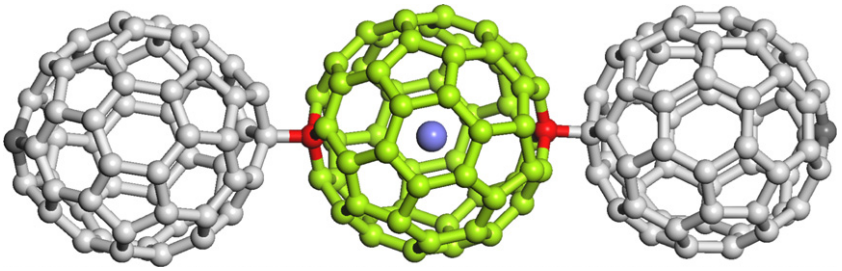

Fig. 1. Structure of single C_{60} molecule centered with one rare gas atom. The gray C_{60} at each side is used to reduce the influence of boundary effect. The gray black denotes fixed particles, the red denotes heat baths. The purple denotes noble gas atom. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The MD simulation is carried out by Verlet algorithm [24], through which the real-time motion can be tracked by integrating the classical motion equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}r_i = \frac{p_i}{m}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}p_i = F_i. \tag{1}$$

The subscript i means the ith particle. r and p are the particle position and momentum, m is the particle mass, F_i is the force applied on the particle, and t is the time. For those particles that are in the heat baths, the momentum equation should be modified to the following equations [25]:

$$\frac{\mathrm{d}}{\mathrm{d}t}p_i = F_i - \Gamma p_i \tag{2}$$

where Γ is the dynamic parameter of the thermostat, which can be determined by the following equations [26]:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma = \frac{1}{Q}\left[\sum_{i=1}^{N_C}\frac{p_i^2}{2m_i} - \frac{3N_C k_B T_0}{2}\right],$$

$$Q = 3N_C k_B T_0 \tau^2/2, \tag{3}$$

in which N_C is the number of atoms in the heat baths, k_B is the Boltzmann constant, T_0 is the set temperature of the heat bath, τ is the relaxation time.

The heat flux is defined as the power injected from the Nose–Hoover thermostat to our system, which is given by

$$J_h = \sum_i \left[-\Gamma p_i^2/m_i\right] = -3\Gamma N_C k_B T\,(t)\,, \tag{4}$$