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Molecular dynamics simulations of noble gases encapsulated in C_{60} Fullerene

W. EVEN†, J. SMITH‡ and M.W. ROTH¶*

†Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803-4001, USA
‡Present address: Sandia National Laboratories, Albuquerque, NM 87185, USA
¶Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614, USA

Molecular dynamics simulations of Helium (He), Neon (Ne), Argon (Ar), Krpton (Kr) and Xenon (Xe) encapsulated in C_{60} are discussed, as well simulations of Fullerenes containing anywhere from two to four He atoms. Even for single atom encapsulates, no species resides at the geometric center of the Fullerene cage. Smaller atoms sit more off-center than larger ones, and He appears to be a special case in both centering and dynamics. Some encapsulated species stabilize the cage by stifling radial fluctuations and others disrupt it; adding Ne seems to have the most stabilizing effect, while Kr and Xe cause the largest radial atomic excursions. Multiple He encapsulates tend to stabilize the cage; such systems are very stressed and show structure over a wide temperature range. Based on dynamical information quadruple He seems to be close to the packing limit for C_{60}.

1. Introduction

Since their discovery nearly 20 years ago, Fullerenes have been of intense scientific interest. Of the many new phenomena presented by systems that include Fullerenes, encapsulation is doubtless one of the most influential and far-reaching. As an example, helium isotopes may be trapped in extraterrestrial objects or even on the ancient earth such that unique isotope ratios of the encapsulated species are preserved and information about the environment or time of formation may be gained [1]. Helium (He), Neon (Ne), Argon (Ar), Krypton (Kr) and Xenon (Xe) have been placed within Fullerenes using either formation in an ambient rare gas environment, high-pressure intrusion, collisions or products of nuclear reactions [2,3]. It was originally a surprise that even Xe could be incorporated into C_{60} [4], as its Van der Waals radius approximates that of the cage vacancy. NMR spectroscopy is used for further study in the cases of ^{3}He and ^{129}Xe [2–4]. The mechanism for encapsulation is still poorly understood. However, utilization of catalyst such as HCN increases incorporation and yield considerably [5], suggesting that the local environment of the Fullerene cage is of considerable importance chemically as well as physically. More than one encapsulated species may be present within a Fullerene cavity, resulting in "molecules" such as He_2 [6], Ne_2 [7] and HeKr [8]. In fact, di-helium [6] has been encapsulated in both C_{70} as well as C_{60}, and has been studied in order to elucidate information about the Fullerene hexanion magnetic fields.

In addition to ongoing experimental efforts, computational studies can lend considerable insight into the dynamical processes exhibited by Fullerene systems. In fact, different mechanisms for encapsulation [2,3] and even release [1] have been proposed and studied computationally [9,10]. Deterministic computer simulations are also used to examine various phase transitions of Fullerenes [11], their melting [12], thermal disintegration [13], fragmentation from collisions [14] and physisorption onto them [15]. Extensive molecular dynamics (MD) simulations of the Fullerene formation process from the vapor phase [16–20] show that monocyclic rings, polycyclic structures and even C_{40}-C_{70} closed cages can coalesce from the carbon vapor phase. In such simulations, a Verlet algorithm is used with temperature control over translational, rotational and

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