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Deterministic Computer Simulations of Noble Gas Disks Orbiting C_{60} Fullerenes

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We present and discuss the results from multiple Molecular Dynamics computer simulations of thermal and mechanical stability of various noble gas discs placed around a central C_{60} fullerene molecule. First thermal stability is evaluated by changing the temperature while holding rotation constant. Without rotation and at low-temperature argon, krypton, and xenon show completely connected discs, while helium and neon have a few symmetric lobes present. As the temperature was increased, the adsorbed layer nearest the fullerene became slightly flatter and the structure furthest away from its center breaks into a larger number of symmetric lobes. With further increase in temperature the system melts, exhibiting diffusion between the lobes and finally the system disintegrates. Second, mechanical stability is studied by changing the angular momentum while holding temperature constant. Rotation causes the adsorbed layer to flatten into a single ring, which orbits the fullerene in a choppy fashion at low angular momentum values. As rotation increases the ring responds by orbiting in a smoother fashion; in addition smaller lobes are produced farther away from the central fullerene. The bulk of the results utilize free boundary conditions but three other types of outer boundary conditions are implemented and the extreme sensitivity of the results to varying boundary conditions is discussed.

Keywords: Fullerenes, Noble Gas, Molecular Dynamics, Orbiting Systems.

RESEARCH ARTICLE

1. INTRODUCTION

Since the discovery of carbon allotropes such as fullerenes[1,2] and nanotubes,[3] scientific interest on the molecular scale has dramatically intensified. Although such small systems exhibit properties unique to their length scale, there are ongoing efforts to simulate nanoscale replicas of devices used in everyday human endeavors such as gears,[4] worm drives[4] and pumps[5]—with the hope of someday being able to manufacture and utilize them. With increasingly robust computational facilities researchers are able to simulate processes seen in biological systems, such as flagellar swimming.[6,7] The comparison of simulated nanodevices with their larger counterparts produces unique results for the particular system.

The largest physical scales known in nature are dominated by gravitational interactions, which are responsible for phenomena ranging from projectile motion to enigmatic patterns possessed by galaxies[8,9] and the superstructure seen in the universe.[10] Although much progress has been made in understanding gravitation and its manifestations, no computational research of nanoscale systems whose forms mirror much larger gravitating systems has been done. One of the main motivations for interest in such modeling is that the atomic/molecular scale forces are uniquely different from gravitation, having different distance dependences. Nanoscale repulsive forces become strongly evident when electron clouds of interacting atoms overlap and have their origin in the Pauli Exclusion Principle. Corresponding attractive (van der Waals) forces have their origin in fluctuating dipolar interactions, and neither nanoscale interaction has a gravitational analog. Another difference between nanoscale and astronomical systems is that the latter mostly involves structures and surfaces which can be approximated as smooth but, when dealing with atoms and molecules the discrete mass and charge distributions must be accounted for in any reasonable model.

Of all the astronomical structures, planetary rings are among the most beautiful and telling of a planet's formation and history.[11] Moreover many aspects of them are not completely understood, such as the appearance of braiding seen in Saturnian ring systems and the presence of rings in our own gas giants and ice giants but apparently nowhere else in the Solar System. Rings represent discrete objects orbiting a smooth planet under conditions of angular momentum conservation and there mere geometry suggests an intriguing nanoscale counterpart.

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