Abstract

This research explores the properties and behaviour of molecules, atoms, and clusters confined within carbon cages, specifically fullerene cages. The study focuses on investigating how confinement within these cages impacts the electronic structure, reactivity, and stability of the systems under consideration. To analyse the properties of confined systems, cutting-edge computational techniques, such as density functional theory (DFT) and molecular dynamics (MD) simulations, are employed. These simulation techniques allow for a molecular-level understanding of the behaviour of confined systems and enable a comparison with the same under isolated conditions.

The study delves into the oxidizing and reducing properties of various systems, including superatoms, within a confined environment. It also explores the influence of confinement size on these properties. Additionally, the catalytic behaviour of computationally designed catalyst is investigated. The research explores the mechanochemical strength of diatomic molecules and examines how it changes within fullerene cages. Notably, the study reveals the distinct behaviour of the Be_3^{2-} system concerning its structure, stability, and aromaticity within a confined environment compared to its isolated state.

The findings of this research contribute to a deeper comprehension of the unique properties exhibited by systems confined within fullerene frameworks. The study highlights how cage interaction influences the electronic structure of confined systems and demonstrates how confinement can either enhance or suppress specific chemical properties. These findings hold significant implications for nanotechnology, materials science, and catalysis applications.

The objectives of this research encompass a broad range of investigations related to the impact of carbon confinement on atomic, molecular, and cluster systems. The goals include understanding the effects of different-sized fullerene cages on electronic properties, studying the catalytic activity of a specific complex, examining the influence of confinement on Fischer and Schrock carbene complexes, investigating the structure, stability, and aromaticity of restricted clusters, and exploring the impact of confinement and external mechanical force on chemical reactions.

Ultimately, this study deepens our understanding of how confinement affects chemical behaviour and provides a foundation for further exploration of confinement-based effects. The insights gained may pave the way for the development of novel materials with desirable properties for various applications, as well as innovative catalysts and strategies for managing chemical processes.

Keywords: Confinement, Cucurbituril, Superatoms, ONIOM, mechanochemistry