

Molecular structure and internal dynamics of endohedral fullerenes: experiment and theory

The term “endohedral fullerene” describes a family of carbon-based cages (fullerenes) hosting atoms, ions or clusters in their inner space.¹ The interaction between the π -system of the carbon cage and endohedral species results in a number of phenomena affecting structural and electronic properties of endohedral fullerenes. When encapsulated species include metal atoms, the electron transfer to the carbon cage takes place with up to 6 electrons formally residing on the fullerene. When more than one metal atom is encapsulated, metal-to-cage electron transfer results in the strong Coulomb repulsion between metal atoms. This destabilizing interaction can be compensated by encapsulation of negatively-charged non-metals, forming so-called clusterfullerenes. The most prominent family of clusterfullerenes are nitride clusterfullerenes $M_3N@C_{2n}$ ($M = Sc, Y, \text{lanthanides}$; $2n = 68-98$). The electron transfer has paramount effect on the molecular structure of EMFs since preferable cage isomer are different for different charge states. The size and the shape of the carbon cage should also fit the size and the shape of the encapsulated cluster. Confinement of the cluster of unsuitable geometrical parameters can result in significant strain, change preferable cage isomer, and even affect electronic and magnetic properties. In this report we will discuss these phenomena on experimental and computational studies.

1. Popov, A. A.; Yang, S.; Dunsch, L. Endohedral Fullerenes. *Chem. Rev.* **2013**, *113*, 5989–6113.