A Computational View of Endohedral Metallofullerenes Chemistry

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Fullerenes containing metals or metallic clusters inside their inner void space, commonly known as endohedral metallofullerenes (EMFs), are very promising nanomaterials with unique properties that might be used in a variety of fields, ranging from molecular electronics to biomedical applications.[1] Due to the complexity of the experimental manipulation and purification of these EMFs systems, computational studies have been shown to be essential for their correct structure elucidation or the study of their properties, for example.[2] In this talk we will review some of the latest and current computational studies carried out in the IQC framework related with the structure and chemical functionalization of EMF species.[3,4] These studies represent a step forward in the understanding of the chemistry and structure of EMFs. Only when we achieve a widely knowledge of fullerene chemistry, we will be able to convert their potential applications into real ones.

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