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Design of nanoporous cluster-assembled materials

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Abstract

Cluster-assembled materials are gaining interest due to their potential applications as nanoporous materials. In addition, interest in metastable solids is raising exponentially as well. The vast amount of possible structures with different properties would lead to new materials with a wide range of applications. In this work we will focus, concretely, on the cluster-assembled structures of II-VI materials, due to their semiconducting properties. The existence of inorganic hollow ZnS and CdS fullerene like clusters was theoretically predicted and then experimentally confirmed recently. These clusters have been predicted to have different metastable cluster-assembled structures, namely, those of FAU, LTA and SOD zeolite-like structures. In addition, the hollow nature of these structures allow for the design of endohedrally-doped building blocks, which would change the properties of the materials according to the dopant material. Concretely, these clusters were seen to trap alkali metals and halogens, being the ionization energies (IE) of the formers very similar to the electron affinities (EA) of the latter. Concretely, we have focused on the assembling of bare $M_{12}S_{12}$ and endohedral $X@M_{12}S_{12}$-$Y@M_{12}S_{12}$ dimers, being M Zn or Cd, X an alkali metal (Na or K) and X a halogen (Cl or Br). In all cases the structures were fully optimized, and their thermal stability was confirmed by ab initio thermal molecular dynamics calculations. Due to their nanoporous structure, these zeolite shaped solids could be used in heterogeneous catalysis, as storage materials and molecular sieves.

Biography

Dr. Jon M. Matxain completed his Ph.D in Chemistry at the age of 26 years, in the Theoretical Chemistry Group at the University of the Basque Country. In this period, he visited the Theory of Condensed Matter Group in Cavendish Laboratory, at the University of Cambridge. He performed postdoctoral studies in the Theoretical Biophysics Group at Örebro University (Sweden). He is a permanent researcher at the University of the Basque Country. He has published about 65 papers in reputed journals.