Novel Solid Phases by Self-Assembling of Nanoclusters

Jon M. Matxain[a]

[a]Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU) and Donostia International Physics Center (DIPC), PK 1072, 20080 Donostia, Euskadi (Spain) e-mail: jonmattin.matxain@ehu.es; ;

Abstract

The theoretical search for novel polymorphs of inorganic compounds have increased significatively in the last years. One of the routes to build such compounds is the so-called nanocluster assembling, where nanometer-sized structures are used as building blocks for the formation of 3D periodic systems. Hollow cage-like structures are ideal candidates for such assembling, resembling the case of carbon fullerenes in fullerites.

In this work we focus on the assembling of bare and endohedrally doped hollow nanoclusters of II-VI materials, concretely, Zn_iS_i and Cd_iS_i, (i=12,16) which were predicted to be the global minima. The considered dopant atoms were several alkali metals, halogens and transition metals [1-3].

Different polymorphs were characterized for all cases [4,5]. Most of them were stable towards vibration. In addition to phonon calculations, quantum molecular dynamics simulations, E vs V calculations were carried out in order to provide some theoretical evidence of the metastability of these compounds. In Figure 1, one of the characterized metastable structure, FAU, is shown.

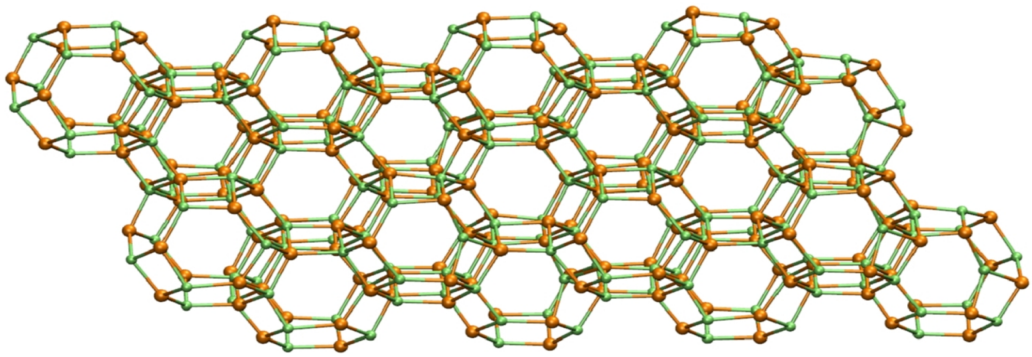

Figure 1: Characterized metastable FAU polymorph build by $Cd_{12}S_{12}$ clusters.

References:

[1] E. Jimenez-Izal, J. M. Azpiroz, R. Gupta, J. M. Matxain, J. M. Ugalde, J. Mol. Model. **20**, (2014) 2227.
[2] E. Jimenez-Izal, J. M. Matxain, M. Piris, J. M. Ugalde, Comput. **1** (2013) 31.
[3] E. Jimenez-Izal, J. M. Matxain, M. Piris, J. M. Ugalde, J. Phys.l Che. C **115**, (2011) 7829.
[4] E. Jimenez-Izal, J. M. Matxain, M. Piris, J. M. Ugalde, Phys. Chem. Chem. Phys. **14** (2012) 9676.
[5] J. M. Matxain, M. Piris, X. Lopez, J. M. Ugalde, Chem. Eur. J. **15** (2009) 5138.