SIMUNE
ATOMISTIC SIMULATIONS

CASE STUDY – CATALYSIS

Azafullerene-like Nanosized Clusters

López, V., Pérez, G. R., Arregui, A., Mateo-Marti, E., Bañares, L., Martín-Gago, J. A., Soler J. M., Gómez-Herrero J. and Zamora, F. ACS Nano, 3, 3352–3357 (2009)

Motivation of the modeling: Carbon nitride materials have extraordinary potential in various applications, including catalysts, filled-particles, and superhard materials. The synthesis and characterization of carbon nitride nanostructures is still a challenge.

Achievements of the model: In this study, computational simulations complement experimental results (XPS, AFM, TEM) on carbon nitride molecules. The structure and stability of new nitrogen-rich carbon nitride nanocages detected by mass spectrometry were characterized using Density Functional Theory calculations (DFT).

Model system/Software: DFT calculations were performed using the **SIESTA** method in order to consider possible structures for the peaks observed in the mass spectra. The stability of the resulting structures was checked by ab-initio Molecular Dynamics (MD).

The SIESTA simulations provided the following main information:

- Formation energy of cluster structures
- Suggestion of cage structures for the new molecules detected by mass spectrometry

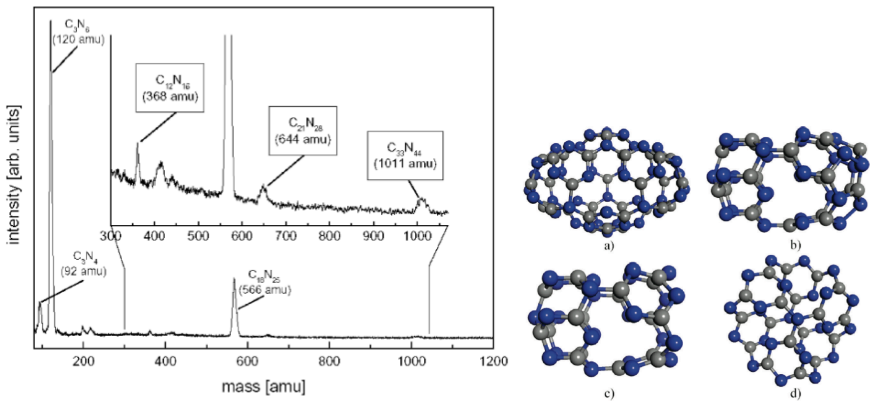

Figure: Left: Mass spectrum measured by laser desorption ionization at 355 nm on a reflectron time-of-flight mass spectrometer of a solid sample obtained by sublimation. The insert shows a magnification of the part of the spectrum corresponding to the larger masses. Right: Proposed graphite C_3N_4 cage-like structures for the peaks observed in mass spectra as result of the SIESTA simulations: (a) $C_{33}N_{44}$, (b) $C_{21}N_{28}$, (c) $C_{18}N_{25}$, (d) $C_{18}N_{26}$. Figures taken from López, V., et. al. ACS Nano, 3, 3352–3357 (2009).

Jose Maria Soler, part of the SIMUNE´s board of experts and member of the core development team of the SIESTA code, is one of the authors of this work.