Abstract/Objectives

The project is devoted to original theoretical and methodological advances that imply a non-routine approach of quantum and computational chemistry. Selecting several important problems we put the accent on conceptual innovation rather than on the exhaustive and quantitative exploration. A first series of objectives concerns the treatment of lanthanide-based endohedral fullerenes by multiconfigurational procedures and subsequent spin-orbit treatments, using original strategies, by assembling a starting wave function from separate fragments. Our treatments enable the realistic description of many effects, paving the way to innovative predictions such as spintronics with lanthanide endohedral fullerenes. Other objectives concern non-metal endohedral fullerene, using a new method to extract host-guest interacting potentials by equating the vibration shifts of the encapsulating host. The same procedure is adapted to systems with tubular topology of the host. The resulting models have relevance for understanding dynamic effects in supramolecular assemblies.

Finally, we focus on planar polyaromatic carbon materials using model Hamiltonians as complement the state of the art calculations. Using spin Hamiltonians and resonance concepts, we treat the spin distribution in triangular and hexagonal distorted graphenes. The polyacenes are taken as molecular models of organic conduction, bringing a fresh perspective in issues with both application relevance and heuristic meaning.

Objectives and activities time-line.

Bonding regime and properties of endohedral fullerenes containing d and f transition metal ions:

-Electron Structure and magnetism in Ln@C82 endohedral systems;

-Electron Structure and stability of Ln@C60 endohedral systems;

-Exchange coupling and dynamic effects in Ln2@C80 and systems with larger cages and nuclearities

Non-covalent interactions in the chemistry of endohedral supramolecular assemblies.

-Non-covalent interactions in noble gas endohedral fullerenes larger than C60;

-Dynamic spectral manifestations in Ng@C60 (Ng=Ar, Kr);

-Supra-molecular interactions in tubular host-guest systems;

Special Properties in Extended Conjugated Carbon Systems. Non-covalent interactions in the chemistry of endohedral supramolecular assemblies.

-Spin coupling, magnetism and resonance effects in triangular graphenes;

-Spin dynamics in distorted hexagonal graphenes;

-Spin Hamilton treatments and conduction models in polyacenes;