

Self-Assembly of Electroactive Systems: From Dimers to Supramolecular Polymers

Enrique Ortí

Instituto de Ciencia Molecular (ICMol), Universidad de Valencia (UVEG), C/ Catedrático José Beltrán 2, 46980 Paterna (Valencia), Spain

Supramolecular aggregates and polymers are macromolecular entities that grow up by the non-covalent interaction of suitable monomeric units. In the search for new materials for optoelectronic applications through self-assembly, the control over the assembly process is one of the most sought-after characteristics. This control is usually achieved by a proper design of the monomeric structure and of the self-assembling motifs (H-bonds, π -stacking, dispersion forces or electrostatic interactions).

The self-assembly of donor-acceptor supramolecular dimers formed by fullerene fragments (buckybowls) and tetrathiafulvalene (TTF)-based electron donors is first described in this presentation. The study relies on theoretical density functional theory (DFT) calculations and illustrates the difficulties in theoretically describing non-covalent interactions. In a following step, the polymerization mechanism and the structural properties of the supramolecular aggregates formed by monomeric units incorporating electroactive fragments are discussed on the basis of theoretical calculations. The discussion includes two types of monomeric units: 1) a bisurea macrocycle bearing electron-donor DMTTF moieties that leads to supramolecular polymers whose self-assembly can be electrochemically controlled, and 2) C_3 -symmetry conjugated systems decorated with peripheral amide groups endowed with paraffinic side chains that form helical π -stacked supramolecular polymers with defined chirality.