FUNDACIÓN RAMÓN ARECES

Summer Course in Nanoscience and Nanotechnology

III "Julio Palacios" International Symposium

A Coruña, 21- 22 July 2022

ABSTRACT

Anions (cations) brought together by non-covalent interactions

Ibon Alkorta

Stable minima showing halogen or hydrogen bonds between charged molecules with the same sign have been explored by means of theoretical calculations. In spite of the ionic repulsion, local energy minima are found both in the gas phase and in aqueous solution. Electrostatic potential and electron density topologies, and the comparison with neutral complexes, reveal that the ionization has no significant effect on the properties of the halogen and hydrogen bonds that hold together the complexes. The stability of the complexes in the gas phase is explained by attractive forces localized in a volume situated in the intermolecular region and defined as the electrostatic attraction region (EAR) and determined by the topological analyses of the electron density and the electrostatic potential, and by the electric field lines. The nature of the interaction in the minima and TSs indicate the presence of local favorable electrostatic interactions in the minima that vanish in the TSs.