Structure andFunctionality of Supramolecular Systems via Ab-initio Calculations

Daniel Sebastiani

Recent progress in both methodologic developments and computer hardware has enabled the direct first-principles based prediction of the physico-chemical properties of condensed-phase systems with hundreds of atoms. Such electronic structure calculations can elucidate the interplay of covalent and non-covalent interactions.

We compute atomistic structure, molecular dynamics and spectroscopic properties of supra-molecular systems. Our aim is to understand the fundamental microscopic processes leading to technologically relevant functionality, in order to provide eventually an approach to a systematic improvement of the related properties.