



Dr. Marco Campetella

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CV

Dr. Marco Campetella has been carrying out his research activity at the Department of Chemistry of the University of Siena since December 2021, previously he carried out his research activity at the CNR of Tor Vergata (Rome), the Sorbonne University of Paris, the Chimie ParisTech of Paris, the Chemistry department of the University of Pisa and the Chemistry department of the "La Sapienza" University of Rome. Dr. Campetella's research activity concerns the calculation and modeling of electronic and structural properties, for the design and characterization of both organic materials (e.g. biological ionic liquids, light harvesting systems) and inorganic materials (e.g. 3D periodic materials -1D, ruthenium complexes, photo-active molecules). For the characterization of structural properties, Dr. Campetella has over the years used existing methodologies, based on a combined approach of experimental and theoretical-computational techniques, and contributed to the implementation of more innovative calculation procedures.

Giovedì 7 Dicembre 2023, h. 16.00

Only online on Team "Seminari Dipartimentali DCCI"

Team code: Iziywqi

Seminar

Automated parameterization of quantum-mechanically derived force-fields including explicit sigma holes: A pathway to energetic and structural features of halogen bonds in gas and condensed phase

Abstract

In classical molecular dynamics, general purpose atomistic force-fields (FFs) often deliver inaccurate results when dealing with halogen bonds (XBs), notwithstanding their crucial role in many fields of science, ranging from material design to drug development. Given the large dimensions of the systems of interest, it would be therefore desirable to increase the FF accuracy maintaining the simplicity of the standard Lennard-Jones (LJ) plus point charge description to avoid an excessive computational cost. A simple yet effective strategy consists in introducing a number of virtual sites able to mimic the so-called "explicit σ -hole." In this work, we present an automated FF parameterization strategy based on a global optimization of both LJ and charge parameters with respect to accurate quantum mechanical data, purposely computed for the system under investigation. As a test case, we report on two homologue series, characterized either by weak or strong XBs, namely, the di-halogenated methanes and the mono-, di-, and tri-substituted acetonitriles, taking into consideration Cl, Br, and I substituents. The resulting quantum mechanically derived FFs are validated for each compound in the gas and in the condensed phase by comparing them to general purpose and specific FFs without virtual sites and to highly accurate reference quantum mechanical data. The results strongly support the adoption of the specific FFs with virtual sites, which overcome the other investigated models in representing both gas phase energetics and the structural patterns of the liquid phase structure related to the presence of XBs.