Seminar
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Online

Dispersion Interactions from the Exchange-Hole Dipole Moment

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Speaker introduction

Alberto Otero de la Roza obtained his Ph.D. in 2011 from the University of Oviedo (Spain) and worked as post-doc in the United States (UC Mercd) and Canada (NINT, UBC) before rejoining the University of Oviedo faculty as a Ramón y Cajal fellow in 2018. His primary field of work is computational chemistry, particularly the development and implementation of methods for non-covalent interactions in density-functional theory. Additional topics of interest are the modeling of materials under extreme conditions of pressure and temperature and the description of chemical bonding in molecules and solids.

Seminar abstract

Non-covalent interactions are ubiquitous in nature. They are essential in the description of the geometry and stability of chemical systems in fields as diverse as supramolecular chemistry, biochemistry, and materials science. Dispersion is an important contribution to non-covalent interaction energies that arises from the correlated movement of electrons on different molecules. The computational modeling of non-covalent interactions and, in particular, dispersion effects, is a field that has experienced enormous progress in the past decade, although a number of important challenges remain. In this talk, I will review computational techniques to the calculation of non-covalent interactions. In particular, I will talk about the exchange-hole dipole moment (XDM) model approach in the context of density-functional theory.

Some applications of XDM include the calculation of:

- molecular crystal stability and phase transitions
- adsorption on metal and mineral surfaces
- pressure-temperature stability and spectra of clathrate hydrates
- enantiomeric excess amplification from lattice energies
- friction on graphite and carbonaceous materials.

One of the challenges in the non-covalent interactions field that remain to be addressed is how to treat large supramolecular systems at a reasonable computational cost. Recent developments on this topic will also be presented.

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