#ICMolTalks

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June 11 · 11:00 h

SS6 Seminario · ICMol

Abstract

What is hidden in a spectrum? Computational strategies from bandshapes to molecular insight

Spectroscopic bandshapes encode detailed information on molecular structure, nuclear motion, electronic-state coupling, environment, aggregation and intermolecular interactions. This molecular information is often hidden in spectral features and is not always straightforward to extract from experiment alone. Computational spectroscopy, which can now provide simulations in direct comparison with experiment, is therefore an ideal tool to reveal such information. To do so reliably, computational models must account for all the relevant physical effects that shape the spectroscopic response.

In this seminar, we will explore computational methodologies developed over the last decade to address different types of spectroscopy. The main focus will be on electronic spectroscopy, including vibronic effects to recover full lineshapes directly comparable with experiment [1]. These techniques can now be routinely applied to semi-rigid systems in heterogeneous environments, provided that the Born-Oppenheimer approximation can be safely invoked for the electronic states involved. For more complex systems, we introduce mixed quantum-classical strategies to treat molecular flexibility and environmental effects on the same footing. In particular, we will discuss the Adiabatic Molecular Dynamics generalized Vertical Hessian (AdMD|gVH) approach [2], a general framework in which harmonic models are generated for stiff solute modes at arbitrary snapshots extracted from unconstrained molecular dynamics simulations. We will review successful applications to flexible chromophores and complex environments [3,4], and discuss the issues arising from non-adiabatic couplings among electronic states, together with different strategies to address them [5,6].

Finally, we will move to infrared spectroscopy and explore the thermodynamics of non-covalent aggregates through the O-H stretching band of phenol. This band is extremely sensitive to aggregation patterns and, therefore, to environmental conditions. We will compare aggregate conformational sampling through systematic searches and molecular dynamics simulations, using a common graph-theory-based classification of aggregate structures [7,8].

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[3] A. Segalina, J. Cerezo, G. Prampolini, F. Santoro and M. Pastore, J. Chem. Theory Comput., 2020, 16, 7061-7077.
[4] J. Cerezo, J. Gierschner, F. Santoro and G. Prampolini, ChemPhysChem, 2024, 25, e202400307.
[5] J. Cerezo, C. Garcia Iriepa, F. Santoro, I. Navizet and G. Prampolini, Phys. Chem. Chem. Phys., 2023, 25, 5007-5020.
[6] A. Schafer, S. Giannini, D. Strelnikov, T. Mohr, F. Santoro, J. Cerezo and M. Kappes, Phys. Chem. Chem. Phys., 2024, 26, 28514-28524.
[7] J. P. Galvez, J. Zuniga and J. Cerezo, J. Chem. Theory Comput., 2025, 21, 3888-3901.
[8] J. P. Galvez, Aggregate, https://github.com/jpablogalvez/Aggregate.

Biography

Javier Cerezo has been an Assistant Professor in the Department of Physical Chemistry at the University of Murcia since October 2025. Previously, he held several positions in the Department of Chemistry at the Universidad Autónoma de Madrid, which he joined in 2017. His work focuses on the computational modelling of photophysical processes in complex environments, developing tools for the simulation of different spectroscopies and for the design of accurate molecular mechanics force fields. These methodologies make it possible to introduce hybrid quantum-classical techniques aimed at simulating the photophysics of systems of biological and technological interest.

He received his PhD from the University of Murcia in 2013 and carried out a postdoctoral stay of almost three years in Dr Fabrizio Santoro's group at the Italian CNR, as well as a short stay at Virginia Tech with Prof Daniel Crawford. He subsequently returned to the Department of Physical Chemistry at the University of Murcia with a talent attraction contract, before rejoining the Universidad Autónoma de Madrid. Throughout his career, he has published around 70 articles, with an h-index of 24, and has delivered more than 20 talks at conferences and seminars, including two invited conference talks. He has also organised a CECAM school in the field of photophysics over the past five editions. He contributes to computational code projects such as FCclasses, a program for the simulation of electronic spectra that is widely accepted by the community, with hundreds of downloads and around 50 citations per year to the article describing it. This article was also recognised with the Award for Methodological Developments from the RSEQ's specialised group on Chemistry and Computation. He is also part of the development team of Joyce, a program for the parametrisation of force fields from QM reference data.