ACCADEMIA NAZIONALE DEI LINCEI E FONDAZIONE «GUIDO DONEGANI»

CONVEGNO LINCEO

LA CHIMICA QUANTISTICA A CENT'ANNI DALL'EQUAZIONE DI SCHRÖDINGER

25-26 MAGGIO 2026

ABSTRACT

Comitato ordinatore: Vincenzo AQUILANTI (Linceo, Università di Perugia), Vincenzo BARONE (Linceo, Scuola Normale Superiore Pisa), Vincenzo SCHETTINO (Linceo, Università di Firenze).

PROGRAMMA

Nel 1926, Erwin Schrödinger, con la formulazione della sua celebre equazione, rese possibile lo sviluppo di tecniche teoriche e computazionali che poterono essere estese alle scienze molecolari, segnando di fatto la nascita della chimica quantistica.

Nei decenni successivi, questi sviluppi accompagnarono—e spesso stimolarono—l'avvento delle scienze informatiche, insieme alle concomitanti applicazioni rivoluzionarie nelle scienze dei materiali e nella biochimica. In quest'ultimo ambito, in particolare, essi hanno contribuito a risultati di grande rilievo, culminati in scoperte premiate con recenti riconoscimenti Nobel.

Il convegno si articola attorno agli sviluppi matematici e formali, nonché agli algoritmi, che hanno reso possibili tali applicazioni. Esso è organizzato in tre principali sezioni tematiche: una prima parte dedicata agli aspetti storici e ai fondamenti teorici; una seconda parte incentrata sulle molecole isolate, con particolare attenzione ai processi elementari e alla reattività in fase gassosa; e una terza parte dedicata alla struttura e alla dinamica molecolare nelle fasi condensate.

Accanto alle relazioni su invito, il programma prevede inoltre contributi aggiuntivi e comunicazioni flash, offrendo ai giovani ricercatori un'importante opportunità per presentare i propri risultati e interagire con la comunità scientifica.

Lunedì 25 maggio

14.30 Carlo DOGLIONI (Presidente della Classe di Scienze Fisiche e Naturali): *Indirizzi di saluto*

Parte 1. Storia e fondamenti

Presiede: Vincenzo AQUILANTI (Linceo, Università di Perugia)

14.45 David C. CLARY (University of Oxford): *Schrödinger, the equation and beyond*

15.15 Cecilia COLETTI (Università di Chieti): *A Momentum-Space View of Schrödinger's Equation: Kepler-Coulomb Orbitals and Hyperspherical Harmonics*

15.40 Eric CANCÉS (École des Pontes): *The electronic Schrödinger equation and its approximations: a mathematical perspective*

16.05 Coffee break

16.30 Kléber MUNDIM (Universidade de Brasília, Brazil): *Beyond the Wave Function: A Schrödinger-Type Equation for Chemical Reaction Rates*

16.55 Sergio RAMPINO (Università di Padova): *At the border between Chemistry and Physics: analysis and interpretation of molecular electron densities with artificial intelligence*

Martedì 26 maggio

Parte 2. Algoritmi e fase gassosa

Presiede: Vincenzo BARONE (Linceo, Scuola Normale Superiore Pisa)

9.00 Loriano STORCHI (Università di Chieti): *BERTHA and PyBERTHA: An HPC-enabled four-component Dirac-Kohn-Sham framework*

9.25 Valter CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil): *Renormalized Chemical Kinetics: Wave-Equation Approach Beyond Mean-Field Behavior in Photochemistry*

9.50 Andrea LOMBARDI (Università di Perugia): *Hyperspherical Molecular Dynamics*

10.15 Coffee break

10.40 Maria Pilar DE LARA-CASTELLS (Consejo Superior de Investigaciones Científicas, Madrid): *After 100 Years of Schrödinger: an Ab initio Journey toward the Molecular-Level Understanding and Predictability of Subnanometric Metal Clusters*

11.05 Dario DE FAZIO (CNR, Montelibretti): *Time dependent quantum reactivity through conical intersections*

11.30 Majdi HOCHLAF (Eiffel Uni, Paris): *Computational spectroscopy: trends from isolated molecules to adsorbed molecules at interfaces and applications*

11.55 Giovanni VILLANI (CNR, Pisa): *Conceptual and Philosophical Aspects of Quantum Chemistry*

12.20 Further and Flash Presentations

Luciano RIBEIRO (Universidade Estadual de Goiás, Brazil): *GSA DVR: Schrödinger Equation Guided Fitting Procedure for Accurate Rovibrational Spectroscopic Properties*

Júlio César O. RIBEIRO (Universidade Federal de Goiás, Brazil): *The Schrödinger Equation Across Scales: Modeling Pesticides and Pharmaceuticals from Mechanisms to Isotopic Signatures*

Parte 3. Dinamica molecolare e fase condensata

Presiede: Vincenzo AQUILANTI (Linceo, Università di Perugia)

14.30 Chiara CAPPELLI (Scuola Normale Superiore di Pisa): *Beyond the Gas Phase: Extending the Schrödinger Equation to Complex Chemical Environments*

14.55 Ilaria CIOFINI (Chimie Paristech-PSL): *Modelling the excited-state properties of molecular systems: from solution to crystals*

15.20 Coffee break

Presiede: Vincenzo BARONE (Linceo, Scuola Normale Superiore Pisa)

15.45 Filippo DE ANGELIS (Università di Perugia): *Quantum mechanics at work: Materials and processes in photovoltaics*

16.10 Matthew GUBERMANN PFEFFER (New Mexico State University): *Quantum Biochemistry*

16.35 *Conclusioni*

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10
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Schrödinger, the equation and beyond

David C. CLARY (University of Oxford)

"We were taken by surprise by Schrödinger's papers on wave mechanics. This was a new approach to quantum mechanics which, at first glance, had no connection with our own work. It was of fascinating power and elegance, and as it used mathematical methods well known to every physicist it quickly became the standard theory."*

*__Max Born__, *My Life. Recollections of a Nobel Laureate*, p. 229 (Taylor & Francis, London, 1978).

This talk will discuss Schrödinger, his equation, and his interactions with quantum chemistry.

For reference:
D. C. Clary, *Schrödinger in Oxford* (World Scientific Publishing, 2022).

A Momentum-Space View of Schrödinger's Equation: Kepler-Coulomb Orbitals and Hyperspherical Harmonics

Cecilia COLETTI (Università di Chieti)

In recent years, Sturmian orbitals have been gaining renewed attention as a promising alternative to the more traditional Slater- and Gaussian-type basis sets in quantum chemistry [1,2]. Their appeal lies not only in their flexibility, but also in a remarkable property: a deep reciprocity between their representation in configuration space and their natural counterparts in momentum space, the hyperspherical harmonics. This duality opens the door to a different way of looking at quantum problems.

Within this perspective, overlap integrals between basis functions can be recast in terms of angular momentum algebra and its generalizations [3], providing a unifying language that connects different Kepler–Coulomb Sturmian bases arising from alternative separations of the hydrogenic Schrödinger equation [4,5]. What may appear as distinct formulations are, in fact, different facets of the same underlying structure. This insight offers a powerful framework for designing basis sets tailored to multielectron and multicenter systems.

The approach is, in principle, dimension independent. It can be extended to a d-dimensional hydrogen atom, although most applications still rely on the familiar three-dimensional case and its associated O(4) hyperspherical symmetry. From this broader viewpoint, the quantum mechanics of atoms and molecules can be interpreted as the progressive breaking of the hyperspherical symmetry of a higher-dimensional hydrogenoid system, with d=3(N-1) for an N-body Coulomb problem, due to the presence of additional charged particles. In this framework, Kepler–Coulomb Sturmian functions provide a natural basis for constructing atomic and molecular orbitals. At the same time, different choices of hyperspherical harmonics, associated with alternative subgroup chains of the (d+1)-dimensional rotation group, offer complementary symmetry-adapted descriptions of the same physical system [6]. This flexibility suggests a route toward more efficient and physically transparent representations of complex quantum systems.

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At the border between Chemistry and Physics: analysis and interpretation of molecular electron densities with artificial intelligence

Sergio RAMPINO (Università di Padova)

The language of chemistry is universally based on simple concepts such as the atom or the bond. Yet, these concepts find no place in a physical description of the molecular world, where – within a Born-Oppenheimer view – a molecule is ultimately represented by a three-dimensional mathematical function expressing the electron density surrounding a given set of nuclei. While several methods have been proposed over the past decades to discern atoms and bonds in the molecular electron density, the search for a universally accepted theory bridging chemical

concepts to the underlying physics is still an open quest. In this contribution, I will discuss to what extent we can harness Artificial Intelligence to trace the physical roots of chemical concepts – from the simple idea of an atom or a bond to more elaborate ones such as the nuanced 'chemistry' of an atom in a given molecular context – and frame these on a quantitative level based on compact numerical representations of the molecular electron densities.

BERTHA and PyBERTHA:
An HPC-enabled four-component Dirac-Kohn-Sham framework
Loriano STORCHI (Università di Chieti)

Loriano Storchi [a,b,c] , Leonardo Belpassi [b]
[a] University of Chieti-Pescara
[b] Istituto di Scienze e Tecnologie Chimiche "Giulio Natta" (SCITEC), CNR, Perugia
[c] INFN (Istituto Nazionale Di Fisica Nucleare) sez. Perugia

This presentation will outline the historical progression of the BERTHA project, a computational code designed for 4-component Dirac-Kohn-Sham (DKS) calculations. BERTHA's development spans several years [1-5], marked by continuous adaptation to advancements in supercomputer architectural hardware. The discussion will encompass initial parallelization strategies, employing MPI and OpenMP, culminating in the complete GPU porting of the code, including the implementation of the Python API known as PyBERTHA. Furthermore, the presentation will offer a quick overview of its diverse applications, notably Real-Time TDDFT and the NOCV/CD approach.

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2. M. De Santis, L. Storchi, L. Belpassi, H. M. Quiney, F. Tarantelli, "PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python", Journal of Chemical Theory and Computation, DOI: 10.1021/acs.jctc.0c00053 (2020).
3. Loriano Storchi, Matteo De Santis, Leonardo Belpassi, "BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations", Advances in Parallel Computing, Parallel Computing: Technology Trends, DOI: 10.3233/APC200060 (2019)
4. Sergio Rampino, Loriano Storchi and Leonardo Belpassi, "Gold-superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study", Journal of Chemical Physics DOI: 10.1063/1.4926533 (2015).
5. Sergio Rampino, Loriano Storchi and Leonardo Belpassi, "Gold-superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study", Journal of Chemical Physics DOI: 10.1063/1.4926533 (2015).

Renormalized Chemical Kinetics: Wave-Equation Approach Beyond Mean-Field Behavior in Photochemistry
Valter CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil)

Complex reactive mechanisms in microscopically nonuniform environments cannot be adequately described by decoupled time and temperature variables. Spatial fluctuations along the reaction pathway may drive the system beyond mean-field behavior and induce an effective thermo-temporal coupling. Here, we introduce a renormalized chemical-kinetics formulation in

which a lumped reactant scalar field evolves in time and reciprocal temperature through coupled first-order partial differential equations. The transitivity function, defined as the reciprocal of the apparent activation energy, mediates this coupling, while the reaction order is generalized to non-integer values. Under isothermal constraint, the formalism reduces to a hyperbolic wave equation that describes nonstationary regimes and emergent apparent kinetic parameters beyond the mean-field limit. Departure from mean-field behavior in spiropyran photochemistry stems a conformational origin, since the thermal evolution of photomerocyanine is governed by the coexistence and interconversion of distinct conformational states. Electronic-structure calculations indicate a more stable trans-like merocyanine structure related to C–N–C–C torsional angle and a less stable cis-like conformer. The transition state for conversion of the cis conformer into closed spiropyran is structurally closer to the cis arrangement, supporting a fast ring-closure step through C–O bond formation. These elementary processes define a minimal mechanistic framework in which conformational variability generates competition between interconversion and reactivity, leading to multiscale and non-exponential behavior. The asymptotic behavior of the coupling parameters in both time and temperature is also examined to identify the limiting regimes controlling the effective mechanistic description. The interconversion toward spiropyran therefore illustrates how conformational variability may provide the physical basis for thermo-temporal coupling in complex photochemical kinetics and how renormalized wave-equation descriptions may help disentangle such mechanisms.

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Hyperspherical Molecular Dynamics

Andrea LOMBARDI (Università di Perugia)

Hyperspherical coordinates constitute a unifying framework for the description of few-body and many-body systems in both quantum and classical mechanics. Originally developed in quantum scattering theory to treat nuclear and molecular collision problems through hyperradial and hyperangular variables (see [1]), the hyperspherical formalism provides a natural representation of collective motions, symmetry properties, and energy redistribution processes. In the quantum framework, hyperspherical harmonics and hyperangular momentum operators define the basis functions and dynamical quantities governing the evolution of the system in configuration space. The hyperradius acts as a collective coordinate measuring the overall size of the system (a natural collision coordinate), while the hyperangles describe its shape and internal rearrangements.

In this contribution, the extension of hyperspherical concepts to classical molecular dynamics is discussed [2], establishing a direct connection with the underlying quantum theory. Starting from the mass-scaled position matrix and its decomposition under ordinary and kinematic rotations, classical analogues of hyperangular momenta and hyperspherical kinetic-energy partitions are introduced. The resulting formulation leads to invariant decompositions of the kinetic energy into hyperradial, rotational, kinematic, and shape contributions, each associated with distinct classes of collective motion. These quantities are instantaneous phase-space invariants and preserve the geometrical interpretation characteristic of the quantum hyperspherical approach.

Numerical investigations on model systems and atomic clusters reveal regular statistical behaviors of the energy partitions, suggesting equipartition-like relations for systems with equal masses and highlighting the role of hyperspherical observables as global indicators of structural transitions. Applications to Lennard-Jones and ionic clusters through caloric curves and energy distributions are presented. The framework also opens perspectives for the analysis of complex molecular systems, including biomolecules and nanostructures, through invariant shape coordinates and deformation descriptors. The parallelism between quantum hyperspherical theory and classical hyperspherical molecular dynamics therefore provides a coherent multiscale language for describing collective dynamics, energy flow, and structural evolution in molecular systems.

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After 100 Years of Schrödinger: an Ab initio Journey toward the Molecular-Level Understanding and Predictability of Subnanometric Metal Clusters

Maria Pilar DE LARA-CASTELLS (Consejo Superior de Investigaciones Científicas, Madrid)

Recent advances in the synthesis and characterization of atomically precise, monodisperse metal clusters (AMCs), composed of just one to ten atoms, are enabling a deeper insight into the physical and chemical nature of matter. Their quantized, "moleculelike" electronic structure endows them with unique stability and properties that differ markedly from those of nanoparticles and bulk materials. When incorporated into materials that interact with environmental molecules and sunlight, AMCs can exhibit enhanced (photo)catalytic activity, as well as distinct electronic and optical properties [1, 2, 8]. In this lecture, state-of-the-art *ab initio* modeling of both free and surface-supported AMCs will be presented, drawing on an overview of recent studies [1–13]. Particular emphasis will be placed on *ab initio* evidence supporting the description of AMCs as fluxional Jahn–Teller systems [1, 5, 11, 12], the influence of AMC–support interactions on associated conical intersections [7], and the role of non-adiabatic effects in their reactivity in O2-rich environments. Finally, recent progress in the *ab initio* benchmarking of density functional theory (DFT) methods for predicting IR and Raman spectra of AMCs will be highlighted, including the effects of anharmonicity and bimetallic intermixing [12, 13].

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Time dependent quantum reactivity through conical intersections

Dario DE FAZIO (CNR, Montelibretti)

Dario De Fazio*[a] and Carlo Petrongolo[b]

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In the last three decades, the development of accurate quantum reactive scattering methods and parallel computer technologies have permitted to solve exactly the time independent and the time dependent Schrödinger's equation for a rearrangement many body problem and to compare different reactive observables with molecular beam experiments, showing the relevance of the quantum mechanics effects on the reactive rearrangement mechanism.

However, the main limit of these ab-initio accurate studies is that nowadays only investigation of simple systems (mainly three-bodies) is computationally feasible, and only particular processes can be studied with both the quantum methods. Therefore, just *ad-hoc* benchmark systems can be compared with experiments to understand the main mechanisms leading to reaction.
Nevertheless, an accurate description of elementary chemical processes is important in many applied environments, as the ones involved in combustion chemistry and astrophysics normally involving many different reactive processes as three-bodies break up dissociation or non-adiabatic effects, still hard to be accurately treated by the theory. Another problem for apply quantum reactive scattering results in chemical evolution models to describe applied systems is that, except in few case, reactive rate constants at high temperatures are required while accurate theoretical investigations are normally achieved just for the ground molecular reactants states. In the conference, I will show the results of a wave packet time dependent code [1] that has been employed successfully to study the conical intersection driven dynamics of the dissociative charge transfer process, namely:

$He^+ + H_2 \rightarrow He + H + H^+$

a non-adiabatic reaction relevant in the Helium chemistry of the early Universe evolution [2] and in different astro-chemistry environments as in the atmosphere escape modeling of Neptune-like exoplanets [3], a class of extragalactic objects fundamental in the description of exoplanet diversity. In particular thermal rate constants have been calculated up to 1000 K and the important role of the reactants vibro-rotational energy has been analyzed [4]. As it is the first time that a dissociative conical intersection reaction has been studied by a quantum reactive scattering method particular effort has been spent to clarify the role of the conical intersection in the reaction dynamics and to understand in detail the resonance mechanism, highly relevant in this range of temperature. The high reaction rate sensitivity to the reactants vibro-rotational states in the hot (up to 5000 K) atmosphere environment could be responsible of recent astronomic observation in the GJ 436 b star, an extragalactic exoplanet deeply investigated in the NASA catalogue

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Computational spectroscopy: trends from isolated molecules to adsorbed molecules at interfaces and applications

Majdi HOCHLAF (Eiffel Uni, Paris)

I will present a comparative study, using first principles methodologies, of the structures and vibrational spectroscopic characteristics of isolated conformers of biofuels such as furfural-acetone-furfural (FAF) [i] and those adsorbed on a Ru(0001) metal surface [ii]. The choice of FAF is motivated by the ease of its synthesis *via* the aldol condensation of furfural with acetone, followed by hydrogenation and hydrodeoxygenation, producing high-value C_8–C_{13} hydrocarbons, [iii,iv] which are components of diesel fuels [v]. Nevertheless, the final steps of the heterogeneous catalysis on the Ru surface are not yet fully understood. Moreover, our work shows that FAF conformers undergo significant structural deformations upon adsorption compared to their structures in the gas phase. Furthermore, the energy order of the conformers is altered upon adsorption. To better understand these adsorption-induced effects, we use various computational descriptors, including adsorption energies, electron density, density of states, and Bader charge analyses.

Besides, I will treat the case of a-carotenes, another biofuel precursors, for which a large conformational landscape exists. [vi] We will use artificial intelligence tools to reduce such large number of conformers to clusters. The reduced number of representatives is then investigated using advanced DFT to compute RAMAN spectra useful to their identification in mixtures. Our strategy is viewed to be cost effective and can be generalized to other medium-sized compounds of organic, inorganic and energy relevance.

This work is conducted in collaboration with Professor R. Linguerri (Université Gustave Eiffel, France), the group of Professor C. Puzzarini (University of Bologna, Italy), and Professor S. Azizi (University of Tlemcen, Algeria). We would like to thank the COST Action CA21101 "COSY – Confined Molecular Systems: From a New Generation of Materials to Stars."

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Conceptual and Philosophical Aspects of Quantum Chemistry

Giovanni VILLANI (CNR, Pisa)

The relationship between quantum chemistry and the conceptual foundations of quantum mechanics is fundamental, yet not always straightforward. In particular, the connections between quantum mechanics, chemical concepts, and their historical development require careful analysis and clarification (Villani, Cubellis 2025). The concept of molecular structure provides a compelling example of this interdisciplinary interplay, which is both productive and complex (Ghibaudi, Cerruti, Villani 2020). While ubiquitous in the chemical literature, this concept poses significant challenges from the standpoint of quantum mechanics (Lombardi, Villani 2024). This presentation offers a historical and epistemological analysis of key chemical concepts and examines their reinterpretation within a quantum framework.

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GSA DVR: Schrödinger Equation Guided Fitting Procedure for Accurate Rovibrational Spectroscopic Properties

Luciano RIBEIRO (Universidade Estadual de Goiás, Brazil)

Luciano Ribeiro[1*], João Paulo Martins[1], Ana Gabriela Coelho Oliveira[2], Heibbe C. B. de Oliveira[2]

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Keywords: *Potential Energy Curve Fitting, Rydberg Function, Schrödinger Equation; Generalized Simulated Annealing; Discrete Variable Representation.*

Abstract

In celebration of the centennial of Schrödinger's equation, we present a hybrid methodology, termed GSA-DVR, for accurately determining rovibrational spectroscopic properties of diatomic molecules. The method combines Generalized Simulated Annealing (GSA) [1] to fit *ab initio* potential energy curves using sixth-order Rydberg

analytical functions [2] with the Discrete Variable Representation (DVR) [3] to solve the nuclear Schrödinger equation and compute rovibrational energy levels. We apply this approach to molecular hydrogen (H_2), its cation (H_2^+), and molecular chlorine (Cl_2) in their ground states and selected excited levels. To enhance accuracy, the GSA cost function is modified to include the experimental harmonic vibrational frequency (ω_e) for each system, ensuring that the fitted potential yields DVR-derived frequencies that closely match experimental data. The resulting GSA-DVR code produces spectroscopic constants and energy levels in excellent agreement with measurements, underscoring the enduring relevance of Schrödinger's equation in modern computational spectroscopy.

Acknowledgments

I thank the State University of Goiás (UEG/PrP) and FAPEG for their essential support in this research.

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The Schrödinger Equation Across Scales: Modeling Pesticides and Pharmaceuticals from Mechanisms to Isotopic Signatures

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The Schrödinger equation provides the conceptual foundation for understanding matter at the molecular scale, and its influence extends across diverse research areas in chemistry. This presentation outlines a research trajectory shaped by that theoretical framework, moving from molecular modeling to environmental and analytical applications. Initial investigations employed density functional theory (DFT) to explore adsorption processes in layered double hydroxides and to analyze reaction mechanisms in hydrolytic systems, emphasizing molecular structure, charge distribution, and thermodynamic stability [1]. These studies highlighted how approximate quantum mechanical solutions inform interpretations of reactivity and environmental behavior. The application of electronic structure methods was further extended to the degradation of emerging contaminants such as ametryn, chlorophenol, sertraline, fluoxetine and others, allowing the elucidation of mechanistic pathways, energetic profiles, and intermolecular interactions. Complementary investigations into non-covalent interaction networks and reaction mechanisms reinforced the role of wavefunction-based approaches in describing weak interactions and transition states in chemically complex systems [2,3,4]. These research directions are particularly relevant in the Brazilian context, where large-scale agricultural production increases the environmental pressure associated with pesticide use and water contamination. In addition, Brazil has experienced a significant rise in the consumption of antidepressants and other psychoactive pharmaceuticals, which are frequently detected as emerging contaminants in aquatic systems. Understanding the degradation pathways and molecular stability of such compounds is therefore essential for assessing environmental persistence, transformation products, and potential ecological impacts. In this setting, combining molecular-level theoretical insight with applied analytical and environmental studies becomes crucial for developing more sustainable monitoring and remediation strategies. In such a setting, combining molecular-level theoretical insight with applied analytical and environmental studies becomes essential for developing more sustainable monitoring and remediation strategies. More recently, quantum chemical calculations have been integrated with high-resolution Orbitrap mass spectrometry to investigate stable isotope fractionation. Vibrational frequency calculations derived from Schrödinger-based formalisms enable prediction of equilibrium isotope and fractionation effects, establishing a direct link between quantum vibrational energies and measurable isotopic ratios such as $\delta^{15}N$ and $\delta^{18}O$. In this context, the Schrödinger equation connects electronic structure theory with analytical isotope science. Across adsorption phenomena, pollutant degradation, non-covalent interactions, reaction mechanisms, and isotope ratio analysis, the Schrödinger equation remains a unifying theoretical framework. A century after its formulation, it continues to guide both predictive modeling and experimental interpretation in contemporary chemical research.

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Modelling the excited-state properties of molecular systems: from solution to crystals

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This contribution will focus on the methods allowing to model the photophysical behavior of molecular systems in condensed phases and their modulation due to aggregation. From a methodological point of view, it will be shown how electrostatic embedding schemes can be applied to accurately model localized excited states in solids by taking into account the electrostatic environment of the crystal, without treating the entire system quantum mechanically. In order to fully recover long-range effects generated by the crystalline environment, we have proposed and applied in the last years the so called “SC-Ewald” approach [1,2] starting from the original work of Derenzo et collaborators [3].

In this contribution it will be shown how such an approach can be used to model the photophysical properties of different systems [4,5] as well as various complex processes (aggregation induced emission,[6] or mechanochromism [7] in molecular crystals). Finally, a Gaussian charge-based (GC) electrostatic embedding scheme will be discussed, as a robust alternative to PC models for excited-state calculations in solids. [8]

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