



ACCADEMIA NAZIONALE DEI LINCEI, FONDAZIONE «GUIDO DONEGANI» E
ACCADEMIA NAZIONALE DELLE SCIENZE DETTA DEI XL

CONVEGNO

QUANTUM CHEMISTRY ONE HUNDRED YEARS AFTER SCHRÖDINGER'S EQUATION

25-26 MAY 2026

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

PROGRAMME

In 1926, Erwin Schrödinger, through the formulation of his celebrated equation, made possible the development of theoretical and computational techniques that could be extended to the molecular sciences, thus marking the birth of quantum chemistry.

In the following decades, these developments accompanied—and often stimulated—the rise of computer science, together with groundbreaking applications in materials science and biochemistry. In the latter field in particular, they led to discoveries that have been recognized with the awarding of recent Nobel Prizes.

The conference is structured around the mathematical and formal developments, as well as the algorithms, that have enabled these applications. It is organized into three main thematic parts: a first section devoted to historical perspectives and fundamental principles; a second section focused on isolated molecules, addressing elementary processes and reactivity in the gas phase; and a third section dealing with molecular structure and dynamics in condensed phases.

In addition to invited lectures, the program also includes further contributions and flash presentations, offering valuable opportunities for young researchers to present their work and engage with the broader scientific community.

Monday, May 25

14.30 Carlo DOGLIONI (Presidente della Classe di Scienze Fisiche e Naturali): *Welcome Address*

I session. History and Foundations

Chair: 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 Estadual de Goiás, Anápolis, Brazil): *Wave equation for kinetics*

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

17.20 Flash Presentations

Tuesday, May 26

II session. Algorithms and Gas-Phase Processes

Chair: Vincenzo BARONE (Linco, Scuola Normale Superiore Pisa)

- 9.00 Lorian STORCHI (Università di Chieti): *Quantum informatics*
- 9.25 Valter CARVALHO (Universidade Estadual de Goiás, Anápolis, Brazil): *Reaction kinetics*
- 9.50 Andrea LOMBARDI (Università di Perugia): *Molecular dynamics simulations*
- 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 methods for 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): *Philosophical aspects of chemical quantum mechanics*
- 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 Estadual de Goiás, Brazil): *The Schrödinger Equation Across Scales: Modeling Pesticides and Pharmaceuticals from Mechanisms to Isotopic Signatures*
- 13.00 Lunch

III session. Molecular Dynamics and Condensed-Phase

Chair: Vincenzo AQUILANTI (Linco, 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 Marco GARAVELLI (Università di Bologna): *Molecular dynamics of excited states*
- 15.20 Ilaria CIOFINI (Chimie Paristech-PSL): *Magnetic systems*
- 15.45 Coffee break
- Chair: Vincenzo BARONE (Linco, Scuola Normale Superiore Pisa)**
- 16.10 Filippo DE ANGELIS (Università di Perugia): *Photovoltaic cells*
- 16.35 Matthew GUBERMANN PFEFFER (New Mexico State University): *Quantum Biochemistry*
- 17.00 *Conclusions*

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10
convegni@lincei.it - <http://www.lincei.it>

All information for participating in the conference is available at:

<https://www.lincei.it/it/manifestazioni/convegno-la-chimica-quantistica-centanni-dallequazione-di-schrodinger>

Online registration is required to attend the conference.
The conference will also be accessible to the public via live streaming.

Access is also possible until 10:00 a.m. from Lungotevere della Farnesina, 10.

A certificate of attendance will be issued only to participants attending in person and must be requested from the staff in the antechamber on the same day of the conference.