

Beyond the Quantum Year: *Theoretical Chemistry Meets the Scuola Superiore Meridionale* QM@SSM

February 4-6, 2026

Aula Magna, Via Mezzocannone, 4 – Napoli

WEDNESDAY, 4 FEBRUARY

9:00 - 9:30 Registration

9:30 - 9:45 Welcome speech

9:45 - 11:15 Session I

Coffee Break

11:45 - 12:55 Session II

Lunch Buffet

14:40 - 15:40 Session III Part A

Coffee Break

16:10 - 16:40 Session III Part B

FRIDAY, 6 FEBRUARY

9:30 - 11:10 Session VII

Coffee Break

11:40 - 13:40 Session VIII

Closing Remarks

THURSDAY, 5 FEBRUARY

9:30 - 10:55 Session IV

Coffee Break

11:25 - 12:55 Session V

Lunch Buffet

14:40 - 15:40 Session VI Part A

Coffee Break

16:10 - 17:05 Session VI Part B

Scientific & Organizing Committee

Nadia **Rega** - Chair - *Scuola Superiore Meridionale*

Paola **Cimino** - *University of Napoli Federico II*

Federico **Coppola** - *Scuola Superiore Meridionale*

Fulvio **Perrella** - *Scuola Superiore Meridionale*

Alessio **Petrone** - *University of Napoli Federico II*

Secretariat

Anna **Citarella** - *Scuola Superiore Meridionale*

Marco **Mesca** - *Scuola Superiore Meridionale*

SSM

Scuola Superiore Meridionale

9:00 – 9:30	Registration
9:30 – 9:45	Welcome and opening speech
... Day 1, 4/02: Aula Magna ...	
Session I – Chair: Nadia Rega	
P. 1 9:45	Benedetta Mennucci - <i>Università di Pisa</i> Photoactivated biological functions: bridging electronic excitations and functional response
O. 1 10:15	Greta Donati - <i>Università di Napoli Federico II</i> Conformational dynamics of bis-(thio)carbohydrazones in a non-protic solvent: a theoretical-computational investigation
O. 2 10:30	Małgorzata Biczysko - <i>Università di Wrocław</i> QM-based approaches for linking protein structure and spectroscopic data
O. 3 10:45	Angela Parise - <i>CNR-IOM / SISSA Trieste</i> Beyond the static structure: decoding the regulatory logic of Rho GTPases via QM/MM and MD simulations
O. 4 11:00	Marco Pagliai - <i>Università di Firenze</i> Improving metalloprotein force fields through quantum mechanical approaches
11:15	Coffee Break
Session II – Chair: Alessio Petrone	
O. 5 11:45	James Cheeseman - <i>Gaussian Inc.</i> Simulation of resonance chiroptical spectra using damped linear response
O. 6 12:00	Massimiliano Aschi - <i>Università dell'Aquila</i> Chirality modulation by external fields: computational insights into environment-driven chiral responses
O. 7 12:15	Julien Bloino - <i>Scuola Normale Superiore di Pisa</i> Anharmonic calculations in routine spectral predictions: a reality?
O. 8 12:30	Andrea Phan Huu - <i>Università di Parma</i> Chirality-induced spin selectivity in photoinduced electron transfer: many-body models and chiral molecular vibrations
O. 9 12:40	Filippo Lipparini - <i>Università di Pisa</i> The importance of polarizable embedding for computing optical rotation
12:55	Light Lunch
Session III Part A – Chair: Federico Coppola	
P. 2 14:40	Anna Painelli - <i>Università di Parma</i> TADF photophysics in condensed phase: liquid vs solid environment
O. 10 15:10	Massimo Olivucci - <i>Università di Siena</i> Photochemistry of an anti-Bredt olefin through the lens of multistate multireference quantum chemistry
O. 11 15:25	Mauro Stener - <i>Università di Trieste</i> New TDDFT algorithms, protocols and analysis tools for the study of optical properties and plasmons of large metal clusters
15:40	Coffee Break
Session III Part B – Chair: Federico Coppola	
O. 12 16:10	Francesco Di Maiolo - <i>Università di Parma</i> Flipping the rules: from inverted singlet-triplet gaps to diradical switches
O. 13 16:20	Prachi Pandey - <i>CNR-ICCOM Pisa</i> Vibronic coupling effects in 9-mesityl-10-methylacridinium cation and its phenyl-derivative: a computational investigation
O. 14 16:30	Xuchun Yang - <i>Università di Siena</i> Protein-controlled excited-state dynamics govern quantum efficiency in visual rhodopsins

Session IV – Chair: Alessio Petrone

P. 3 9:30	Giovanni Scalmari - <i>Gaussian Inc.</i> Stability, CIS/TDA, and TD for complex and general HF/KS-SCF
O. 15 10:00	Carlo Adamo - <i>Chimie ParisTech - PSL University</i> Are standard benchmarks enough for reliable DFT?
O. 16 10:15	Ciro Achille Guido - <i>Università del Piemonte Orientale</i> Quantum chemistry simulation of circularly polarized luminescence: from linear response to real-time approaches
O. 17 10:30	Stefano Russo - <i>Scuola Superiore Meridionale</i> Molecular simulations of locally concentrated electrolytes
O. 18 10:40	Ivan Carnimeo - <i>SISSA - Scuola Internazionale Superiore di Studi Avanzati</i> Excited-state forces in periodic systems
10:55	Coffee Break

Session V – Chair: Fulvio Perrella

O. 19 11:25	Martina Stella - <i>ICTP - International Centre for Theoretical Physics</i> Quantum simulations of molecular excitations in photoactivated drugs
O. 20 11:40	Marta Erminia Alberto - <i>Università della Calabria</i> Using computational approaches to explore how light-activated processes trigger anticancer responses in photoactivated therapeutic agents
O. 21 11:55	Isabella Daidone - <i>Università dell'Aquila</i> Intermolecular photoinduced electron transfer in biosystems: impact of conformational transitions and multiple channels on kinetics
O. 22 12:10	Ivan Rivalta - <i>Università di Bologna</i> Generating molecules with artificial intelligence without databases
O. 23 12:25	Emilia Sicilia - <i>Università della Calabria</i> Computational chemistry tools for anticancer activity prediction of transition metal complexes as photoactivated chemotherapy agents
O. 24 12:40	Tiziana Marino - <i>Università della Calabria</i> Advancements in enzyme modeling: some studied cases
12:55	Light Lunch

Session VI Part A – Chair: Federico Coppola

P. 4 14:40	Ilaria Ciofini - <i>Chimie ParisTech - PSL University</i> Electrostatic embedding schemes for the description of excited-state properties of crystalline materials
O. 25 15:10	Fortuna Ponte - <i>Università della Calabria</i> From theoretical chemistry to oncology: mechanistic and photophysical insights into Ru(II)-based compounds for PACT cancer therapy
O. 26 15:20	Massimo Christian D'Alterio - <i>Università di Napoli Federico II</i> From structure to function: noncovalent interactions directing poly(cyclohexene carbonate) organization and enantioselective catalysis
O. 27 15:30	Francesca Fasulo - <i>Università di Napoli Federico II</i> Interfacial structure and charge dynamics in advanced solar energy conversion devices: a first-principles perspective
15:40	Coffee Break

Session VI Part B – Chair: Federico Coppola

O. 28 16:10	Francesca D'Ambrosio - <i>Università di Roma "La Sapienza"</i> Unraveling structure–property relationships in carbon nanodots: a computational challenge
O. 29 16:20	Pietro Maria Curzietti - <i>Scuola Normale Superiore di Pisa</i> Theoretical study of the adsorption of polycyclic aromatic hydrocarbons on [010] Epsomite and [100] Hexaydrite (MgSO ₄ (H ₂ O) _n , n = 7,6) surfaces

O. 30 16:30	Alfonso Pedone - <i>Università di Modena e Reggio Emilia</i> Machine learning interatomic potentials for napso glass electrolytes: opportunities and limitations of universal models
O. 31 16:45	Filippo Sacchetta - <i>Università di Siena</i> Rhodopsin charge diffusion computations disclose contrasting color-tuning mechanisms
O. 32 16:55	Francesco Calcagno - <i>Università di Bologna</i> Quantum computers for molecular inverse design: the quantum ensemble variational optimization algorithm

... Day 3, 6/02: Aula Magna ...

Session VII – Chair: Fulvio Perrella	
P. 5 9:30	Cristina Puzzarini - <i>Università di Bologna</i> From quantum chemistry to astrochemistry: modeling reactivity under interstellar conditions
P. 6 10:00	Jingjing Zheng - <i>Gaussian Inc.</i> Study of spectrum and nonadiabatic reaction using Ring-Polymer Ehrenfest dynamics method
O. 33 10:30	Nicola Tasinato - <i>Scuola Normale Superiore di Pisa</i> In silico assessment of climate metrics
O. 34 10:45	Mario Prejanò - <i>Università della Calabria</i> Reactivity and enantioselectivity in enzymes: opportunities and current challenges for modelers
O. 35 11:00	Silvia Alessandrini - <i>Università di Bologna</i> Formation of glycolamide (NH ₂ C(=O)CH ₂ OH) on interstellar ice grains: insights from atomistic simulations
11:10	Coffee Break
Session VIII – Chair: Nadia Rega	
P. 7 11:40	Angela Violi - <i>University of Michigan</i> NeCLAS: A domain-agnostic machine learning protocol for bridging scales in nanoscale interactions
O. 36 12:10	Gabriele D'Avino - <i>Università Ca' Foscari Venezia</i> Modeling record-mobility organic semiconductors: vibrations, electrons, transport
O. 37 12:25	Andrea Correa - <i>Università di Napoli Federico II</i> Multiscale molecular modeling of methanol sorption in glassy polyetherimide
O. 38 12:40	Raoul Carfora - <i>Scuola Superiore Meridionale</i> Photoinduced vibrational relaxation pathways in molecular rotors revealed by ab initio molecular dynamics and Wavelet analysis
O. 39 12:50	Enrico Bodo - <i>Università di Roma "La Sapienza"</i> Modelling electrolytes with high-accuracy force fields: recent developments
O. 40 13:05	Anna Piras - <i>CNR-ICCOM Pisa</i> Development of QM-derived force fields for small molecules adsorbed in porous materials
O. 41 13:15	Giovanni Di Liberto - <i>Università di Milano-Bicocca</i> Understanding single-atom catalyst with quantum chemical simulations: new properties, reactivity and beyond
O. 42 13:30	Pierpaolo D'Antoni - <i>Università di Trieste</i> Efficient Hybrid Diagonal Approximation to speed up accurate TDDFT calculations on large systems
13:40	Closing Remarks

P: Plenary speaker
O: Oral contribution