ACCADEMIA NAZIONALE DEI LINCEI E FONDAZIONE «GUIDO DONEGANI»

CONFERENCE

QUANTUM CHEMISTRY AND CHEMINFORMATICS

26-27 SEPTEMBER 2024

ROME PALAZZO CORSINI - VIA DELLA LUNGARA, 10

Comitato ordinatore: Vincenzo AQUILANTI (Linceo, Università di Perugia), Vincenzo BARONE (Linceo, Scuola Normale Superiore Pisa), Sergio CARRÀ (Linceo, Politecnico di Milano), Cecilia COLETTI (Università di Chieti-Pescara), Laura GAGLIARDI (Lincea, University of Chicago), Gianfranco PACCHIONI (Linceo, Università di Milano Bicocca), Giorgio PARISI (Linceo, Sapienza Università di Roma), Vincenzo SCHETTINO (Linceo, Università di Firenze), Roberta SESSOLI (Lincea, Università di Firenze), Antonio SGAMELLOTTI (Linceo, Università di Perugia), Adriano ZECCHINA (Linceo, Università di Torino)

ANNOUNCEMENT

One century ago, at the birth of quantum mechanics, Dirac claimed the discovery of the founding laws of chemistry, as the science of materials at the atomic and molecular level -- however admitting that the challenge to full application needed development of efficient computational techniques. The following decade recorded the birth of information science (Von Neumann and Wigner were among founding fathers of both sciences): progress and implementations to chemistry became instrumental and today mature: Quantum Chemistry explains and predicts a variety of new phenomena, occurring in the rarefied situations of the planetary atmospheres and of the interstellar medium, and including those relevant for thermal and non-equilibrium plasmas; emerging tasks are imposed to biochemists, instrumental to life and health sciences; research is active on the electro-magnetic properties of solid conductors and semiconductors for optoelectronic applications; current Holy Grail is the chemical hardware to support exploitation of Quantum Computing. Physicochemical models at micro, meso and macro scales allow one to accumulate myriads of data that can be handled through cheminformatics approaches for the scrutiny of properties of materials or molecules, both exploiting through powerful Machine Learning methods to obtain otherwise unavailable information and to highlight through Artificial Intelligence technology correlations and universalities of behavior otherwise hidden in the non-linear equations of current complexity theory.

Thursday, 26 September

14.00 *Welcome addresses from the Presidency of the Academy*

14.15 Vincenzo AQUILANTI (Linceo, Università di Perugia), Cecilia COLETTI (Università di Chieti-Pescara): *Introduction*

Session I – Chair: Cecilia COLETTI (Università di Chieti-Pescara)

14.30 Peter M.W. GILL (University of Sidney, Australia): *Parsimonious descriptions of molecular orbitals*

15.00 Roland LINDH (Uppsala Universitet, Sweden): *Bye-bye to second-order optimization methods*

15.30 Gianfranco PACCHIONI (Linceo, Università di Milano Bicocca): *40 years in quantum chemistry: from Li clusters to nanocatalysis*

16.00 Break

16.20 Anna KRYLOV (University of Southern California, Los Angeles, USA): *In Search of Molecular Hardware for Quantum Information Science: A Quantum Chemistry Perspective*

16.50 Sonia CORIANI (Technical University of Denmark, Lyngby, Denmark): *Ab initio modeling the molecular response to light: from ultrafast (local) spectroscopy to quantum computing*

Friday, 27 September

Session II – Chair: Niyazi BULUT (Firat University, Elazig, Turkey)

9.20 Ireneusz GRABOWSKI (Nicolaus Copernicus University, Torun, Poland): *A Comprehensive Assessment of Hybrid Kohn-Sham DFT Functionals*

9.50 Valter H. CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil): *Ascent and Decline in the Temperature Dependence of Rate Processes for Biophysical Systems*

10.20 Michele CEOTTO (Università di Milano): *Unraveling Water Solvation Effects with Quantum Mechanics/Molecular Mechanics Semiclassical Vibrational Spectroscopy*

10.50 Break

Session III – Chair: Vincenzo BARONE (Scuola Normale Superiore di Pisa)

11.10 Joel M. BOWMAN (Emory University, Atlanta USA): *Permutationally Invariant Polynomial Regression is Perhaps The Fastest and Most Precise Machine Learning Method for High Dimensional Molecular Potentials*

11.40 Leonardo BELPASSI (CNR-SCITEC Perugia): *Relativistic Quantum Chemistry: past, present and future*

12.00 Loriano STORCHI (Università G. d'Annunzio, Chieti-Pescara): *Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator*

12.20 Dario DE FAZIO (CNR Montelibretti): *Artificial Quantization: Discrete Harmonics Algorithm for QRS*

12.35 Flavio Olimpio SANCHES-NETO (Instituto Federal de Educação, Ciência e Tecnologia de Goiás): *Mechanisms and Kinetics of Environmental Biocomplexity: A Quantum Chemistry and Machine Learning Perspective*

12.50 Break

14.00 Pier Luigi GENTILI (Università di Perugia): *An Unconventional Chemical Approach for the Development of Quantum Artificial Intelligence*

14.20 Alberto BAIARDI (IBM Zurich, Switzerland): *Development of Quantum Computing Algorithms for Quantum Chemistry Simulations*

14.50 Markus MEUWLY (Universitat Basel, Switzerland): *Machine Learning Models and Applications for Chemical Reactions*

15.20 Andrea LOMBARDI (Università di Perugia): *Machine learning oriented approach to few-and-many-body systems by hyperspherical coordinates and harmonics*

15.50 Hamilton BARBOSA NAPOLITANO (Universidade Estadual de Goiás): *Chalcone compounds as alternatives for fuel additives: from solid state analysis to machine learning protocols*

16.20 *Conclusions*

The conference, that involves no participation fee, is particularly convenient for international travelers bound to Italy through Rome airports. It is part of the Days on *One Hundred Years of Quantum Chemistry* and follows the *Molecular Electronic Structure* event (https://www.mes2024.it/) that will take place in Pescara from 21 to 25 September 2024 Transportation from Pescara to Accademia in Rome will be arranged in the morning of September 26.

The sessions will start from after lunch on the 26th and end on the 27th at 17 p.m. *Besides the talks already programmed, according to demand, further short presentations and/or poster exhibitions can be arranged.*

The location, among the most prestigious in Trastevere, in the heart of Rome, enjoys an ample variety of accommodations at any level, but the most convenient need early booking: some suggestions will be provided. The Accademia guesthouse for speakers and chairpersons will be granted for free on a first serving basis. Free parking will be available.

ROMA - PALAZZO CORSINI - VIA DELLA LUNGARA, 10
Conference secretariat: convegni@lincei.it – https://www.lincei.it

Information to participate in the conference will be uploaded and updated on the Lincei website:

https://www.lincei.it/it/manifestazioni/quantum-chemistry-and-cheminformatics-convegno

Online registration is necessary to attend the conference

Fino alle ore 10 è possibile l'accesso anche da Lungotevere della Farnesina, 10
I lavori potranno essere seguiti dal pubblico anche in streaming

L'attestato di partecipazione al convegno viene rilasciato esclusivamente a seguito di partecipazione in presenza fisica e deve essere richiesto al personale preposto in anticamera nello stesso giorno di svolgimento del convegno