



ACCADEMIA NAZIONALE DEI LINCEI E FONDAZIONE «GUIDO DONEGANI»

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CONVEGNO

# QUANTUM CHEMISTRY AND CHEMINFORMATICS

## CHIMICA QUANTISTICA E INFORMATICA CHIMICA

26-27 SETTEMBRE 2024

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### ANNOUNCEMENT

One century ago, at the birth of quantum mechanics, Dirac claimed the discovery of the basic principles 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, mandatory 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, and physicochemical models at micro, meso and macro scales allow one to accumulate myriads of data -- they can be only handled through cheminformatics approaches to the scrutiny of properties of materials or molecules; both exploiting powerful Machine Learning methods to obtain otherwise unavailable information and to reveal, through Artificial Intelligence approaches, the hidden correlations and universalities of behavior, otherwise obscure in the non-linear equations of current complexity theory.

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 26<sup>th</sup> and end on the 27<sup>th</sup> at 17 p.m. About 15 talks will be programmed. According to demand, 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.

Conference secretariat: [convegni@lincei.it](mailto:convegni@lincei.it)

Information to participate in the conference will be uploaded and updated on the Lincei website. -  
<http://www.lincei.it>