Quantum Chemistry Meets Artificial Intelligence to Understand Complex Molecular Processes across Biology, Materials, and Cultural Heritage

Thursday, March 26th, 2026
11:00

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and on TEAMS:
https://teams.microsoft.com/meet/35096542593233?p=bTGHDJzXjhCmAtJTPu

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Abstract

Understanding complex molecular processes requires bridging accurate molecular-scale descriptions with chemically relevant models applicable to real systems. In this seminar, I will show how the integration of **quantum chemistry and artificial intelligence** provides a coherent framework to address this challenge across biomolecular systems, functional materials, and cultural-heritage-related compounds.

The talk will start from **small- to medium-sized molecules** as essential building blocks for the construction of reliable, chemically meaningful databases. These datasets enable the development of **continuous, chemically based molecular descriptors**, designed to explore chemical spaces of manageable size while retaining physical interpretability. High-level **gas-phase quantum-chemical calculations**, combined with **high-resolution rotational and vibrational spectroscopy**, will be presented as a key strategy to disentangle intrinsic molecular properties from environmental effects.

Building on this reference picture, the role of **intermolecular interactions**, **bulk effects**, and **molecular dynamics in solution** will be discussed to rationalize how realistic environments modify structure, energetics, and spectroscopic observables. Finally, I will illustrate how **virtual reality and immersive visualization tools** can connect microscopic molecular information to macroscopic behavior, providing an intuitive bridge between theory, experiment, and applications.

https://it.wikipedia.org/wiki/Vincenzo_Barone