

Welcome Seminar

14 Novembre 2024 - h15:00
Aula A

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Ricercatore a tempo
determinato di tipo B

Dipartimento di Scienze Chimiche
Università degli studi di Padova

Chemistry with Computers: from Interstellar Processes to Solvated Macromolecules through HPC, Virtual Reality and AI

The past few decades have witnessed relentless progress in information and communication technology that has pushed the interaction of Chemistry and Computer Science well beyond the traditional aspect of scientific computing. In this talk, I will draw from my past and present research activity to highlight how novel paradigms such as High Performance Computing (HPC), Virtual Reality (VR) and Artificial Intelligence (AI) can be beneficially integrated in Chemistry. Applications include the dynamics of astrochemical reactions, the analysis of chemical bonding in coordination complexes, the relativistic chemistry of superheavy elements, and the description of flexibility of macromolecules in solution. I will conclude by illustrating the work that I am undertaking within the Theoretical Chemistry Group in Padua on several venues for the integration of AI and Chemistry, including the development of a deep-learning framework for the analysis and interpretation of molecular electron densities.

