POLITECNICO
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DIPARTIMENTO DI CHIMICA,
MATERIALI E INGEGNERIA CHIMICA
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Development and Application of Quantum Chemistry and Quantum Crystallography Methods

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Introduction, prof. **Piero Macchi** (Politecnico di Milano, DCMIC)

25 November 2021 | 16:00

Aula Luca Bertolini
Via Mancinelli 7, Milano

live | online

link will be emailed to
registered participants

Registration Form

Quantum crystallography is an emerging field of science with the goal of investigating properties and phenomena of the crystalline state that can be explained only through the laws of quantum mechanics.[1] To accomplish this task, several methods have been developed over the years.[2] They range from the traditional multipole model techniques for the determination of experimental electron densities from X-ray diffraction data to the more recent X-ray restrained wavefunction (XRW) approach and Hirshfeld atom refinement (HAR), which are characterized by an even stricter relationship with usual quantum chemistry methods[3]. In this seminar, the connection between quantum chemistry and quantum crystallography will be highlighted by reviewing some of the techniques recently developed in my research group.

In the first part of the presentation, I will describe quantum chemistry techniques conceived for the treatment of large (bio)systems and based on the use of extremely localized molecular orbitals (ELMOs), which are molecular orbitals strictly localized on small molecular fragments and easily transferable from a molecule to another. Particular attention will be given to two methods: i) the ELMO libraries[4] for the instantaneous reconstruction of approximate wavefunctions and electron densities of macromolecules (e.g., proteins); ii) the recently proposed QM/ELMO multiscale embedding approach[5] for the accurate treatment of chemically relevant regions of macromolecules.

In the second part, the focus will shift towards modern methods of quantum crystallography, showing how concepts and techniques presented in the first part of the seminar were also successfully exploited to propose more advanced quantum crystallographic techniques. Three methods will be briefly overviewed: i) the X-ray restrained ELMO-Valence Bond (XR-ELMO-VB) approach[6] for the determination of resonance structure weights from X-ray diffraction data; ii) the HAR-ELMO technique[7] for quantum chemistry-based refinements of macromolecular crystal structures; iii) the ELMO-embedded HAR strategy,[8] where the above-mentioned QM/ELMO method has been exploited to improve the performances of the popular Hirshfeld atom refinement in case of crystal structures characterized by strong intermolecular interactions.

Future perspectives and next development steps will be also discussed.

References:

[1] P. Macchi, Crystallogr. Rev. 26, 209-268 (2020).
[2] A. Genoni, L. Bučinský, N. Claiser et al., Chem. Eur. J. 24, 10881-10905 (2018).
[3] S. Grabowsky, A. Genoni, H.-B. Bürgi, Chem. Sci. 8, 4159-4176 (2017).
[4] B. Meyer, A. Genoni, J. Phys. Chem. A 122, 8965-8981 (2018).
[5] G. Macetti, E. K. Wieduwilt, A. Genoni, J. Phys. Chem. A 125, 2709-2726 (2021).
[6] A. Genoni, Acta Cryst. A 73, 312-316 (2017).
[7] L. A. Malaspina, E. K. Wieduwilt, J. Bergmann et al., J. Phys. Chem. Lett. 10, 6973-6982 (2019).
[8] E. K. Wieduwilt, G. Macetti, A. Genoni, J. Phys. Chem. Lett. 12, 463-471 (2021).

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