POLITECNICO
MILANO 1863

DIPARTIMENTO DI CHIMICA,
MATERIALI E INGEGNERIA CHIMICA
GIULIO NATTA

Quantum Crystallography: where synergistic interplay between experiment and computation takes place

Dr. Giovanni Macetti
(Department of Chemistry, Università degli Studi di Milano)

15 December 2023 | 14:30

Aula Bertolini | DCMIC
Via Mancinelli 7, Milano

live | online

link will be emailed to registered participants

Registration Form

Since their inception, crystallography and quantum mechanics have shared an intimate relationship, paving the way to the emergence of the quantum crystallography discipline [1]. Intended in the broadest sense, quantum crystallography is a field of science aimed at investigating properties of the crystalline state exploiting the laws of quantum mechanics. To achieve this goal, several methods have been developed over the years [2-3]. Despite their diversity, these techniques share a common foundation: the exploitation of the synergistic interplay between quantum mechanics and crystallography.
The initial part of this seminar will provide a comprehensive introduction to quantum crystallography and will present its main techniques. Particular attention will be devoted to two distinct categories of methods. Firstly, I will discuss the techniques that leverage quantum calculations to enhance the accuracy of the experimental results, for example the Hirshfeld atom refinement [4]. Subsequently, I will explore methods capable of embedding information obtained from experimental data into molecular wave functions or density matrices, as illustrated by the X-ray restrained/constrained wave function approach [5].
The second part will concentrate on modern quantum crystallography methods that have been developed within my research group over the last years [6-7]. These techniques center around the use of extremely localized molecular orbitals (ELMOs) [8]. which are orbitals strictly localized on small molecular fragments. Due to their inherent transferability, these orbitals are especially useful for describing large (bio)molecules and polymers. The novel QM/ELMO-based techniques will also be discussed in detail [9].
In conclusion, the seminar will explore future perspectives and potential advancements in the field, underscoring once again the importance of combining experimental and theoretical approaches to fully unlock the potential inherent in both realms.

References:

[1] P. Macchi, Crystallogr. Rev. 2020, 26, 209-268.
[2] A. Genoni, L. Bucinksy et al., Chem. Eur. J. 2018, 24, 10881-10905.
[3] A. Genoni, P. Macchi, Crystals 2020, 10, 473.
[4] D. Jayatilaka, B. Dittrich, et al., Acta Cryst. A 2008, 64, 383-393.
[5] D. Jayatilaka, Phys. Rev. Lett. 1998, 80, 798-801.
[6] E. K. Wieduwilt, G. Macetti, A. Genoni, J. Phys. Chem. Lett. 2021, 12, 463-471.
[7] G. Macetti, P. Macchi, A. Genoni, Acta Cryst. B 2021, 77, 695-705.
[8] B. Meyer, A. Genoni, J. Phys. Chem. A 2018, 122, 8965-8981.
[9] G. Macetti, A. Genoni, J. Phys. Chem. A. 2021, 125, 2709-2726.

More info: www.cmic.polimi.it