UNIMORE Dipartimento di Scienze Fisiche, Informatiche e Matematiche
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

CNRNANO MODENA S3

FIM-S3 SEMINAR

Modeling Molecular Crystals with Machine Learning Interatomic Potentials

Tuesday September 9th, 2025 – 11.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building
Remote link: Teams

Speaker

Ivor LONČARIĆ – Ruđer Bošković Institute, Croatia

Abstract

Molecular crystals are a common and important class of crystalline materials. However, modelling molecular crystals based on first principles (eg. with density functional theory) is often difficult due to the size of a typical unit cell. Therefore, high-throughput calculations for the discovery of useful properties are rare. In this presentation, I will show how machine-learned interatomic potentials can enable accurate and fast calculations of mechanical and thermal properties of molecular crystals, enabling an understanding of experimental observations as well as a high-throughput search for materials with the desired properties [1,2,3,4]. In principle, to train machine learning potential, one would need to create a sufficiently large database of molecular crystals calculated with the desired accuracy. This is also a very challenging task, and we will show how to avoid this step using transfer learning and existing databases of small systems.

[1] Ivan Žugec, R. Matthias Geilhufe, and Ivor Lončarić. "Global machine learning potentials for molecular crystals." The Journal of Chemical Physics 160, 15 (2024)
[2] Bruno Mladineo and Ivor Lončarić. "Thermosalient phase transitions from machine learning interatomic potential." Crystal Growth & Design 24, 20, 8167–8173 (2024)
[3] Hunnisett, Lily M., et al. "The seventh blind test of crystal structure prediction: structure ranking methods." Acta Cryst. B 80, 6 (2024)
[4] Anastasiia Kholtobina and Ivor Lončarić. "Exploring elastic properties of molecular crystals with universal machine learning interatomic potentials." Materials & Design 114047 (2025)

Host: Raffaello Bianco

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