# Modelling Amorphous Materials with Machine Learning Interatomic Potentials

**Onurcan Kaya**[1], Stephan Roche[1]
*Catalan Institute of Nanoscience and Nanotechnology*
onurcan.kaya@icn2.cat

## Abstract

Understanding the microscopic properties of materials is increasingly important for establishing precise links between fabrication conditions and the resulting properties and performance in applications. Quantum-mechanical atomistic simulations, mainly density functional theory (DFT), have provided important insights into the atomic structure of disordered materials, but they are computationally expensive and can only describe complex systems in small model sizes. Machine learning interatomic potentials trained on quantum-mechanical data are a rapidly emerging approach that overcomes this limitation, achieving comparable accuracy while giving access to much larger-scale simulations.

In this talk, I will present a machine learning interatomic potential framework trained for non-crystalline materials using an efficient workflow that relies on pre-trained foundational model MACE-MP-0 [2]. The workflow uses foundational models to generate diverse atomic configurations through melt-quench molecular dynamics, which are then labelled with DFT to obtain forces and energies for the training dataset. I will demonstrate the workflow on amorphous carbon and amorphous boron nitride compounds, training both GAP [3] and MACE [4] potentials. Using the resulting potentials, I generate realistic structural models of these disordered systems and investigate their atomic-scale properties, including short- and medium-range ordering in the disordered networks. I will compare the simulated structures against experimental observables such as diffraction patterns and structure factors. Using large-scale simulations inaccessible to DFT, I will present the morphology of the resulting amorphous networks and their mechanical and elastic properties, and discuss the structure-property relationships in these disordered systems. This established workflow provides a scalable method to generate accurate atomistic models for complex disordered materials and directly links their simulated configurations to macroscopic experimental data.

## References

[1] Bartok, A., et al., Science Advances, 3 (2017) e1701816.
[2] Batatia, I., et al., The Journal of Chemical Physics 163 (2025) 18.
[3] Bartok, A., et al., Physical Review Letters 104, (2010) 136403.
[4] Batatia, I., et al., Advances in Neural Information Processing Systems (2022).