Learning Structure–Property Relations Across Quantum, Porous and Molecular Materials

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This talk presents recent and ongoing work at the interface of machine learning, condensed matter physics, topological data analysis, and materials modelling, with a focus on physically motivated representations for learning structure–property relations across quantum, porous, and molecular materials.

The first part concerns magnetic anisotropy energy in transition-metal dimers on defected graphene. I will discuss machine learning models trained on DFT data, the use of orbital-resolved densities of states as spectral representations, and ongoing work with recurrent neural networks for modelling the relation between electronic spectra and magnetic anisotropy energy.

The second part addresses porous materials. I will present direction-aware topological descriptors — filtrations anchored to spatial directions — used for predicting elastic constants and thermal transport in nanoporous metals. I will also discuss neural surrogates for flow fields in porous media, including pressure-dependent flows and a tailored loss function for reconstructing physically relevant flow patterns.

The third part concerns superconductivity in high-entropy alloys. I will describe an active-learning loop coupling fast KKR-CPA electronic-structure calculations with Bayesian optimisation to explore bcc multi-principal-element alloys, with experimental validation of selected compositions.

Overall, the talk highlights how physics-adapted representations can support accurate and interpretable models across different classes of materials..