PAUL SCHERRER INSTITUT

LMS Seminar

Wednesday, March 30, 2022, 14:00-15:00 OSGA/EG05

From the electronic-structure genome to autonomous materials discovery

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Abstract:
The discovery of novel materials and their deployment in devices is empowered by a powerful combination of materials theory and understanding, with automated and autonomous simulations and experiments. Here I will present three case studies illustrating this vision. 1) A microscopic picture of ferroelectric perovskites, obtained merging symmetry analysis together with first-principles combinatorial simulations, to elucidate their hidden-order dynamics and the nature of order-disorder transitions. 2) A comprehensive charting of the electronic-structure genome of all known inorganic materials: I will describe our recent developments to obtain, in an unsupervised approach, reduced-order Hamiltonian representations of materials, and then discuss examples of how these can enable accelerated discovery (e.g. for thermoelectrics), as well as autonomous characterization via a powerful combination of simulations and robotic experiments. 3) The systematic determination of the spectroscopic fingerprints (infrared and Raman) of any multilayer, based on an exhaustive symmetry analysis of the low-frequency shear and layer-breathing modes, then made available as an accessible open tool on the Materials Cloud portal, to enable the vibrational recognition of van-der-Waals heterostructures by the experimental community. These examples illustrate the power and the promise of open digital infrastructures integrating simulations, artificial intelligence and autonomous laboratories as enablers driving computational materials science to the next decade.

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