Let them learn: AI models that master materials physics

Michele Ceriotti[1]

[1] École Polytechnique Fédérale de Lausanne, Switzerland

Machine learning is transforming the way we perform simulations to predict and understand the properties of materials. Traditional "physics-informed" models build symmetry, smoothness, and other physical priors into the mathematical structure of the model to guide learning. In this talk, I'll explore how much physics we really need to include when teaching machines the quantum behavior of matter. I'll contrast models constrained by physical assumptions with emerging, unconstrained approaches that learn physical relationships directly from data. These models can reach, and sometimes exceed, the accuracy and efficiency of their physics-based counterparts, though they require some care to avoid unphysical results. I'll illustrate these ideas using PET-MAD, a lightweight, data-driven model that learns across the periodic table, providing accurate predictions of the microscopic properties of materials that include a quantification of the model uncertainties, both against the reference electronic-structure calculations, and against experiments.