Machine-learning for molecular materials

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Over recent years machine-learning (ML) approaches have prominently found their place in the physical and biological sciences — whether it is as surrogate models promising chemically-accurate, atomic-scale properties predictions for complex systems (while sidestepping much of the computational cost of first-principles methods), or as a means of performing data-driven classifications and extracting important physical insight into the structure-property relations of materials.
I will argue that exploiting fundamental symmetries in the description of atomistic systems facilitates effective ML for materials and very briefly introduce recent methodological developments in the context of symmetry-adapted density-based approaches.
I will then highlight their potential by outlining recent applications to molecular materials, including an assessment of approximate free energy methods, accounting for molecular flexibility in determining the stability of amino-acids, and predictions of NMR chemical shieldings for molecular crystals.
Finally, I will present an example of how ML can be beneficial for the complex tasks of identifying stabilisable phases among databases of (computationally) locally-stable atomic structures.