Advances in machine learning for materials modelling

Advances in machine learning methods for the prediction of structures and properties of materials

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Looking past the hype, machine learning (ML) has made significant contributions to our ability to both predict the structure and properties of materials at significantly larger time and length scales than was possible but a few years ago. In addition, the modelling of complex phenomena that are computationally demanding and could until recently only be applied to a few cherry-picked examples, can now be accelerated to the point of being able to perform high-throughput screening. Unlike the advances being made in ML outside the physical sciences which come in large part thanks to using more compute and larger amounts of training data, much of the progress in ML for materials has come from injecting more physical insights and carefully constraining models to respect physical laws that we know should or must hold. In this vain, this mini-symposium is designed to stimulate discussion and exchange on two aspects of the growing use of ML for materials modelling:

1. advancements in methods and tools that enhance our ability to understand the structure-property relationship, and,
2. applications that demonstrate new possibilities enabled by ML.

Examples of the former can include:

- advancements in the accuracy and transferability for machine learning interaction potentials,
- surrogate models that accelerate electronic structure calculations,
- prediction of experimental quantities (e.g. NMR, Raman, adsorption spectra, etc),
- inverse design/generative models that can predict structures directly,
- unsupervised methods that can help find patterns and understanding in computational or experimental materials' data,
- while examples of the latter include:
- the study of materials by ML accelerated molecular dynamics or enhanced sampling including defects, dislocations, interfaces, etc,
- ML assisted high-throughput screening,
- disordered systems and high-entropy alloys,
- optical, non-trivial magnetic and topological properties of materials.

These lists are by no means exhaustive and we aim to bring together a broad community of developers and users of ML for understanding materials within France and beyond.