AI in Materials Modelling: A Game Changer?

Volker Eyert

Materials Design SARL, 42 avenue Verdier, 92120 Montrouge, France, veyert@materialsdesign.com, www.materialsdesign.com

Key Words: *Machine Learning, Machine-Learned Potentials, Multiscale Simulations, Expert Systems*

Abstract

We are currently witnessing an explosion of AI-related tools with an unprecedented impact not only on our life and our societies but also on our scientific practices and understanding. While in general, AI draws its power from the accumulation and digestion of huge amounts of data from all domains of human life, in materials research, AI is turning the page from physics-based to data-driven approaches exploiting especially a huge amount of measured and calculated materials data. As a consequence, future successful tools for materials research will need the capability to collect data and to generate new knowledge from them. In fact, AI in the physical sciences is not new and our company has pursued the combination of data and simulations for over a quarter of a century. For example, expert systems using databases of measured physical or chemical data allow us to identify new materials with dedicated properties while excluding, e.g., environmentally detrimental or poisonous materials. Similar strategies can be applied to calculated data and have recently initiated the transition from computing materials properties directly from ab initio simulations to approaches using a database of precalculated ab initio data for the generation of machine-learned potentials (MLPs), thereby opening the horizon to investigate larger models at longer time scales. Common to these tools is a qualitative change of the way we access and understand materials properties [1].

This talk will illustrate the recent development of modern software systems towards AI-guided materials research with examples from the MedeA computational environment of Materials Design. These include the Polymer Expert module as an expert system for polymer science, which enables generating new polymers with tailored properties from a large database of repeat units. In contrast, the MLP Generator uses large training sets of ab initio data to generate machine-learned potentials for use, e.g., in large-scale molecular dynamics simulations. The presentation ranges from a discussion of the basic concepts to challenges in creating efficient training sets and practical applications of MLPs to the calculation of properties, which benefit from the extended length and times scales offered by forcefield calculations. The talk will close with an outlook on current trends such as universal MLPs and MLPs for generalized structure-property relations.

References

[1] V. Eyert, J. Wormald, W. A. Curtin, and E. Wimmer, *Machine-learned interatomic potentials: Recent developments and prospective applications*, J. Mater. Res. **38**, 5079 (2023); Overview article of a Focus Issue on *Machine-learned Potentials in Materials Research*, J. Mater. Res. **38**(24) (2023).