Machine learning approaches provide interatomic potentials with DFT accuracy: tungsten and iron as examples

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Abstract

Approximating first principles electronic structure methods by interatomic potentials cannot be avoided for the simulation of materials in order to reach the length and time scales necessary to describe many mechanical and thermodynamical and processes. In this talk, I will review our work in the last few years in applying high dimensional fitting approaches, inspired by the "machine learning" and statistical modelling. The resulting potentials are free of fixed functional form, and can in principle approach the Born-Oppenheimer potential energy surface with sufficient training data. The cost of such simulations is orders of magnitude larger than using e.g. simple EAM potentials, but have similarly favourable scaling and are many orders of magnitude faster than explicit *ab initio* molecular dynamics.

References

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