From Machine-Learning Interatomic Potentials to Atomic-Scale Materials Science

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Understanding the links between structure and properties in materials is one of the most central challenges for computational physics, chemistry, and materials science. Atomic-scale simulations based on density-functional theory (DFT) have played important roles in this – but they are computationally expensive and can describe structurally complex materials only in small model systems. Novel interatomic potentials based on machine learning (ML) have recently garnered a lot of attention in computational physics, chemistry, and materials science: these simulation tools achieve close-to DFT accuracy at only a fraction of the cost.

In the first part of this talk, I will argue that ML-based interatomic potentials are particularly useful for studying materials with complex structures, such as amorphous (non-crystalline) solids. I will describe an ML potential for amorphous carbon **[1]** that was built using the Gaussian Approximation Potential (GAP) framework **[2]**, with a special view on what is needed to create and validate ML potentials for the amorphous state. I will present recent applications of GAP-ML models to porous and partly "graphitised" carbons that are relevant for batteries and supercapacitors **[3]**, and to amorphous silicon, where ML-driven simulations allowed us to unlock long simulation times and accurate atomistic structures **[4]**.

In the second part, I will point out possible directions for the automated exploration and "learning" of condensed-phase potential-energy landscapes. We have recently introduced an ML-driven approach to inorganic crystal structure prediction, dubbed GAP-driven random structure searching (GAP-RSS) **[5]**. This technique, iteratively exploring and fitting structural space, allowed us to create to a flexible and accurate interatomic potential for elemental boron **[5]**, and more recently to develop a more general computational framework that can explore and fit potential-energy surfaces for different materials **[6]**. These early results are hoped to enable a more widespread use of ML-driven materials simulations in the years to come.

References

1. V. L. Deringer and G. Csányi, *Phys. Rev. B* **95** (2017), 094203.
2. A. P. Bartók, M. C. Payne, R. Kondor, and G. Csányi, *Phys. Rev. Lett.* **104** (2010), 136403.
3. V. L. Deringer, C. Merlet, Y. Hu, et al., *Chem. Commun.* **54** (2018), 5988.
4. V. L. Deringer, N. Bernstein, A. P. Bartók, et al., *J. Phys. Chem. Lett.* **9** (2018), 2879.
5. V. L. Deringer, C. J. Pickard, and G. Csányi, *Phys. Rev. Lett.* **120** (2018), 156001.
6. N. Bernstein, G. Csányi, and V. L. Deringer, arXiv:1905.10407.