

Machine learning local atomic properties within the Gaussian approximation potential framework

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Molecular dynamics (MD) simulations are a useful tool to understand the interactions between atoms and to get insight into the processes that take place at the nanoscale and give rise to the observed properties of materials. "Classical" interatomic potentials, based on i) harmonic description of bonds, ii) partial electrostatic charges and iii) Lennard-Jones approximations for dispersion interactions, are computationally efficient but do not grant accurate representation of the real underlying physics/chemistry. They tend to fail at flexibly describing molecules in changing environments, especially when there is bond rearrangement, i.e., when chemical reactions take place. Density functional theory (DFT), on the other hand, offers a satisfactory description of interatomic interactions and can be used to characterize bond formation and annihilation. Unfortunately, DFT becomes prohibitively expensive when running MD of systems beyond a few hundreds of atoms or for time scales longer than a nanosecond. To bridge this gap between computational efficiency and accuracy, algorithmic developments that make use of machine learning techniques are being adopted by the community. In particular, the Gaussian approximation potential (GAP) framework [1] is becoming increasingly popular to describe interatomic interactions in the form of cohesive, or "total", energies. However, GAP-type interpolation can be used, in principle, also to learn local atomic properties other than total energies. Adsorption characteristics and spectroscopic signatures of atoms are possibly the most relevant examples. In this presentation, I will introduce a new method to predict adsorption energies, with an example application to amorphous carbon surfaces [2] (although the method is general). I will also present a new type of atomic descriptor which allows us to improve the predictive ability of GAP models and therefore bring them closer to full DFT accuracy [2]. If time allows, I will also discuss ongoing work on machine learning of x-ray spectroscopic signatures within the GAP framework.

[1] A.P. Bartok, M.C. Payne, R. Kondor, G. Csanyi, *Phys. Rev. Lett.* **104**, 136403 (2010).

[2] M.A. Caro, A. Aarva, V.L. Deringer, G. Csanyi, and T. Laurila, *Chem. Mater.* DOI: 10.1021/acs.chemmater.8b03353 (2018).