MACHINE LEARNING OF SURFACE ADSORBATE STRUCTURE

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The adsorption and self-organisation of molecules at inorganic surfaces is central to many industrial processes from catalysis and coatings, to organic electronics and solar cells. Since structure determines function, any computational study of pertinent processes first requires knowledge of the interface morphology. To efficiently search many atomistic configurations on large length scales, we developed a parameter-free machine learning tool for exploring organic/inorganic interfaces. Our preferred Bayesian optimisation approach [1] relies on probabilities to construct model functions, which are then iteratively refined by input of real data points balancing exploitation with exploration. A Bayesian optimisation algorithm was interfaced with both classical potential and density-functional theory codes to enable iterative learning (on-the-fly) of potential energy surfaces (PES) on large supercomputers without human input. For additional efficiency, the method exploits structural rigidity of molecular groups, reducing the degrees of freedom and making the learning process analogous to "molecular LEGO".

We present a proof-of-concept test based on the alanine molecule (Figure 1) and an application featuring electron donor C_{60} molecules on the (101) surface of TiO_2 anatase. The Bayesian optimisation structure search (BOSS) acquires PES information fast and is particularly efficient in pinpointing the global minimum structure. This versatile scheme for global minimum search could be extended beyond interface packing considerations to address complex configurational problems across scientific disciplines.

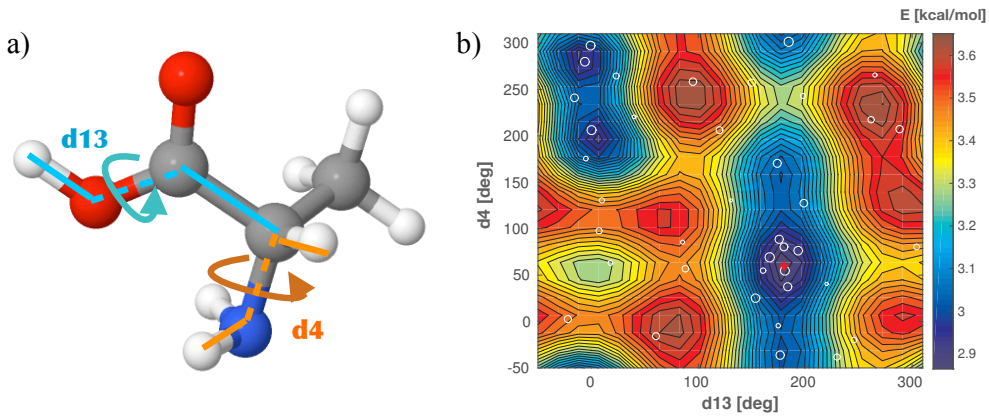

Figure 1: a) Illustration of two dihedral angles of the amino acid alanine; b) Corresponding potential energy map learned by BOSS after only 30 acquisition points.

[1] M. U. Gutmann and J. Corander, arXiv:1501.03291, stat.ML (2015)