Accurate simulation of high-dimensional potential energy surfaces using artificial neural networks

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The aim of this project is to assess the accuracy of a machine learning (ML) method recently developed in our group [1] for the computation of potential energy surfaces of molecules. The method will be benchmarked on a data set, containing energies and forces of thousands of geometries of several organic molecules (Benzene, Uracil, Naphthalene, Aspirin, Salicylic acid, Malonaldehyde, Ethanol, Toluene) computed with Density Functional Theory (DFT) [2–4].

Determining molecular properties is central in chemistry. A common choice to compute such properties are *ab initio* methods, which are accurate but computationally expensive. A cheaper alternative is provided by machine learning algorithms which are becoming more and more popular tools in chemistry and physics. These algorithms can be trained to predict a given molecular property with the accuracy of *ab initio* methods. The choice of input features, adequately representing the molecular geometry and composition, is crucial to train the ML algorithm. A new set of input features was proposed in our recent work [1]. This promising method, which achieves high accuracy in the prediction of molecular energies, has so far been applied only to the acetone molecule. Further benchmarking is therefore required.

The results of this project will provide an extensive benchmark study of the ML algorithm recently developed in our group, and thus open up the possibility for its application in molecular dynamics simulations and for the calculation of various molecular properties.

[1] B. Casier *et al.*, J. Chem. Phys. **152**, (2020).

[2] K. T. Schütt *et al.*, Nat. Commun. **8**, 13890 (2017).

[3] S. Chmiela *et al.*, Sci. Adv. **3**, e1603015 (2017).

[4] S. Chmiela *et al.*, Nat. Commun. **9**, 3887 (2018).