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Machine Learning Methods for the Sampling of Chemical Space From First Principles

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Computational brute force high-throughput screening of compounds is beyond any capacity for all but the most restricted systems due to the combinatorial nature of chemical space, i.e. all the compositional, constitutional, and conformational isomers. Efficient computational materials design algorithms must therefore make good trade-offs between the accuracy of the applied model and computational speed. Overall, rapid convergence in terms of number of compounds visited is highly desirable. In this talk, I will describe recent contributions in this field based on statistical approaches that can serve as inexpensive surrogate models to reduce the computational load of quantum mechanical calculations. Such surrogate machine learning (ML) models infer quantum mechanical observables of novel materials, rather than solving approximate variants of Schroedinger's equation. We developed accurate ML models for the rapid prediction of atomization energies and enthalpies, cohesive energies, and electronic properties that conventionally can only be predicted using quantum mechanics. All our ML models have been trained using large data bases containing properties of thousands of chemical compounds and materials. I will exemplify our approach for the prediction of properties from scratch for out-of-sample compounds. These predictions reach quantum chemical accuracy and are basically instantaneous, i.e. at a computational cost reduced by several orders of magnitude.

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