Universität Basel

Research Project

Sampling chemical space with alchemical perturbation theory

Third-party funded project

Project title Sampling chemical space with alchemical perturbation theory
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Much research is devoted to the study of the relationship between the properties of materials and their chemical composition and structure. Rigorously rooted in quantum mechanics (QM), statistical mechanics, and heavy computing, employed methods nowadays permit to routinely predict relevant properties for novel combinations of atomic configurations and composition, effectively sampling chemical compound space (CCS). The task of using QM for the discovery of novel compounds with improved properties is therefore equivalent to a combinatorial optimization problem in CCS. Albeit straight-forward, tackling this task through QM based high-throughput screening is the least efficient way. This proposal is about the advancement of methods which enable the exploration and sampling of CCS in dramatically more efficient ways, without loss of accuracy. In particular, we plan to use “alchemical” perturbation theory which leverages differential, response-like, QM calculations of reference molecules and materials. Results for these perturbation theoretical calculations can subsequently be usedto accurately estimate properties of thousands, if not millions, new molecules and materials “close by” in CCS with negligible, or constant, computational overhead. Building on recent contributions, we propose three sub projects: (1) to investigate alchemical second and higher order perturbations to afford potential energy estimates of molecules with unprecedented speed and accuracy. (2) to use alchemical estimates for the tailoring of electronic properties in novel materials (important for renewable energy applications),and (3) to make accurate alchemical estimates of chemical reaction energy profiles (important for improved reaction conditions or catalysts).

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