Universität Basel

Research Project

Machine learning models of solid properties for high-throughput screening of condensed phase materials with chemical accuracy

Project funded by own resources

Project title Machine learning models of solid properties for high-throughput screening of condensed phase materials with chemical accuracy
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Organisation / Research unit
Departement Chemie / Physikalische Chemie (Lilienfeld)
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The high-throughput screening of large databases of novel materials candidates constitutes a central goal of the Materials Genome Initiative (MGI). In previous work we have shown that given a training set of molecules with pre-calculated quantum mechanical properties, supervised machine learning models can be constructed that infer corresponding properties for other molecules with quantum chemical accuracy (10 meV error). When compared to quantum mechanical calculations, these estimates can be made at a computational cost reduced by several orders of magnitude. Given sufficient CPU time, this approach could be used for multiple property optimization runs that visit thousands, if not millions of compounds. We propose to develop this approach so that it can be applied to the high-throughput screening of novel condensed systems. If successful, the resulting impact on atomistic simulation methodology as well as computational materials design can be hardly overstated.

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