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The Quantum Machine: Supervised Learning of Schrödinger's Equation in Chemical Compound Space

Dr O. Anatole von Lilienfeld
Argonne Leadership Computing Facility
Argonne National Laboratory

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Abstract: It is a timely goal in the biological and materials sciences to computationally design novel compounds that exhibit specific chemical properties, and are straightforward to synthesize. Some of the most relevant and promising materials properties depend explicitly on atomistic details, rendering an atomistic resolution of any employed simulation model mandatory. Alas, even when using high-performance computing, brute force high-throughput screening of all the possible compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical compound space (compositional, constitutional, and conformational isomers). Consequently, when it comes to properties or systems that require first principles calculations, a successful optimization algorithms must not only make a trade-off between sufficient accuracy of applied models and computational speed, but must also aim for rapid convergence in terms of number of compounds "visited". I will present recent contributions related to the former aspect, namely kernel ridge regression and neural network models that permit rapid prediction of electronic structure properties (atomization energies, HOMO/LUMO, polarizability, excitation energies) for novel compounds with an accuracy similar that goes beyond typical density functional theory. I will also discuss necessary and desired requirements of compound descriptors, and strategies for the generation of training data.