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Quantum Machine Learning

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Many of the most relevant properties of matter depend explicitly on atomistic detail, rendering a first principles approach mandatory. Due to the combinatorial scaling of possible compositions and structures this precludes systematic high-throughput screening in search of new compounds for all but the simplest system classes and properties. Therefore it is desirable to exploit implicit redundancies, present in repeatedly performed quantum calculations. I will discuss our latest machine learning models of quantum mechanical observables, trained and applied throughout chemical compound space.