Quantum Machine Learning

A talk by Anatole von Lilienfeld

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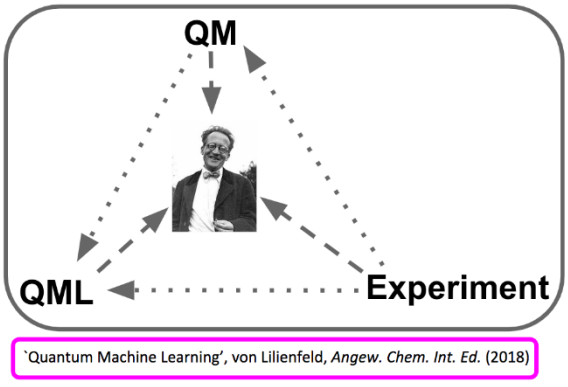
DATE / TIME: Monday, 10th of December 2018, 04:00 p.m.

LOCATION: TU Vienna, Seminar Room 138C (Freihaus, Tower B/yellow, 9. OG)

Many of the most relevant chemical properties of matter depend explicitly on atomistic and electronic details, rendering a first principles approach to chemistry mandatory. Alas, even when using high-performance computers, brute force high-throughput screening of compounds is beyond any capacity for all but the simplest systems and properties due to the combinatorial nature of chemical space, i.e. all compositional, constitutional, and conformational isomers. Consequently, efficient exploration algorithms need to exploit all implicit redundancies present in chemical space.

I will discuss recently developed statistical learning approaches for interpolating quantum mechanical observables in compositional and constitutional space. Results for our models indicate remarkable performance in terms of accuracy, speed, universality, and size scalability.



`Quantum Machine Learning', von Lilienfeld, *Angew. Chem. Int. Ed.* (2018)