Machine Learning meets First Principles towards a Periodic Table of Materials

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First-principles algorithms are now powerful enough that they can predict many properties of materials and molecules before they are synthesized. By implementing and developing new approaches to calculate materials and chemical properties in supercomputers, we have predicted over hundreds of thousands of materials for condensed matter physics and renewable energy.

The computations predicted several new materials which were made and tested in the lab. The creation of our large amount of materials *in-silico*, has prompted us to create our own type of materials Atlas for different purposes. We have implemented different machine learning methods to find further (materials or transition) design principles.

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