Optimization of Catalysts with virtual High Throughput Screenings, Genetic Algorithms, and Machine Learning

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Recent success of advanced atomistic computational chemistry in predicting chemical reactivity, or materials properties, rendered them a valuable and accepted means to tackle problems in academia and nowadays in industry. The development of new simulation methods and new computer architectures enables an enormous improvement of the productivity of research and development of new chemical synthesis.
Approaches like virtual high throughput screenings are highly scalable and allow a deep and very fast insight into the impact of new promising system modifications. These improvements can be accessed with much less time, material, and staff. Thus, the time to application and risk of new synthesis development can be decreased significantly.
The field of computational chemistry is diverse and offers a number of inherently different approaches suitable for different problems, targeting isolated molecules in the gas phase to extended solids, polymers and liquids. Simulating not only energy and derivative properties, but adding a time domain to the problem, accesses the dynamics of the system of interest. New methods are enabling the access to molecular level morphology and dynamics of a materials and catalysts, which can have a crucial impact on activity and stability.
We present the application of modern quantum mechanics in chemical reaction analysis/optimization. We show how hundreds, or thousands of new reactions or material derivatives can be investigated in few days at high accuracy with virtual high throughput screenings and modern optimization algorithms. We present how material morphology and dynamics looks like on atomic level, and what we can learn from that new insight. As well we show how machine learning research is reaching the research and development in chemistry.
Finally, we present how two recent R&D projects in conventional catalysis and electro catalysis leads to two new patents, starting from the simulation approach and keep the focus only on the promising experiments within a few months.