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Exploiting a Tripartite Alliance of Computational Chemistry, Cheminformatics and Machine Learning for Computer-Aided Catalyst Discovery

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Catalysis plays a huge role in the chemical industry as almost every chemical process utilized to produce household, industrial and consumer products requires the use of a catalyst. Hence, the discovery and/or development of new catalysts is a very active field with various experimental strategies/techniques employed, including synthesis, spectroscopic characterization, and reaction optimization. Although computational chemistry methods allow a speedy implementation of this process, the rise of Chemoinformatics as well as machine learning techniques in chemistry in recent years, in addition, have created a pathway to accelerate this discovery process even further. Hence in this talk, I will present how a tripartite alliance of these three methods – computational chemistry, chemoinformatics and machine learning can be explored to search for more active catalysts for important chemical processes using non-heme Fe(II) alkane oxidation catalysts as a case study.

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