Computational and Machine Learning Studies of Homogeneous Catalysis

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Abstract

Computational science is an enabling technology capable of accelerating growth and for offering detailed insights into problems in a given domain of research. For instance, computational quantum chemistry has been increasingly employed toward rationalizing the stereochemical outcome of catalytic reactions.[1] In our laboratory, density functional theory computations are employed to gain insights into stereoselective reactions of immediate practical significance.[2] The key objective of our research is to decipher the factors responsible for stereoselectivity and to harness such knowledge toward *in silico* design of novel asymmetric catalysts.[3]

In general, the presentation would encompass a few contemporary themes in the domain of asymmetric multi-catalytic reactions.[4] The process of chirality transfer from the catalysts to the developing stereogenic center(s) in the product could be understood with the help of our computed transition state for the enantio/diastereo-controlling step in the catalytic cycle. In keeping with the latest developments in multidisciplinary research, we have been trying to tap the potential of machine intelligence for chemical catalysis. An overview of how machine learning models, built on intuitively chosen molecular descriptors, could be exploited in asymmetric catalysis as a way to develop high-throughput methods will also be presented.[5]

References

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