DATA-DRIVEN PREDICTIONS OF ORGANIC REACTIVITY AND SELECTIVITY

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Abstract

Quantum chemical models of reaction mechanism and selectivity provide a powerful tool to explain the outcome of laboratory experiments. However, since many reactions involve several steps and multiple conformers, the computational expense of QM approaches often prevent their application to predict reaction outcomes more broadly. Surrogate machine-learning models with quantum chemical accuracy at a fraction of the computational cost are set to transform the accessibility of computational predictions of reactivity and selectivity. I will discuss machine learning efforts utilizing knowledge and data from QM studies to generate surrogate models for the large-scale prediction of various atomic and molecular properties. We have developed graph neural networks to predict computational and experimental observables such as spin density, chemical shift, thermochemistry and reactivity. In this talk I discuss the performance of these models in high-throughput predictions of reactivity and selectivity of heteroaromatics and in goal-directed molecular optimization of stable organic radicals, along with strategies to improve model transferability.

Bio: Dr. Robert Paton is a Professor of Chemistry and the inaugural holder of the Marshall Fixman and Branka Ladanyi Professorship at Colorado State University. Research in the Paton group is focused on the development and application of computational tools to accelerate chemical discovery. Paton has received the Harrison-Meldola Medal of the Royal Society of Chemistry (RSC), an Outstanding Junior Faculty Award from the ACS Computers in Chemistry Division, the Silver Jubilee Prize of the Molecular Graphics and Modeling Society and is a Fellow of the RSC. The Paton group enjoy collaborative research and are members of the NSF Center for Computer-Assisted Synthesis (C-CAS), the NSF Molecular Maker Lab Institute (MMLI), and the Center for Sustainable Photoredox Catalysis.