SOCIÉTÉ CHIMIQUE DE GENÈVE

Predicting chemical reactivity using digital tools

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Chemistry is often described as the science of matter and its changes. One important type of change is chemical reactions, which transform chemical compounds into new ones. Controlling chemical reactivity has allowed an unprecedented rise in human welfare over the last two centuries, exemplified by the Haber-Bosch process and synthesis of fine chemicals such as drugs and pesticides. While such control has in the past been achieved by laborious experimentation, it has in the last few decades been aided by computer simulations. Over the last decade, machine learning has started to become useful for reaction prediction and promises to greatly accelerate discovery of new catalysts.

In this talk, I will outline our work in "digital chemistry", an emerging interdisciplinary research field which uses methods from cheminformatics, computational chemistry and machine learning to accelerate chemical discovery. While our tools are computers, we work closely with experimental colleagues in academia and industry to make sure that our methods are practically useful. I will give examples of reaction prediction in the pharmaceutical industry for smarter drug synthesis. To do this, we need both data and some way for the computer to understand what a molecule is. We gather this data both from the academic literature, but also create simulated datasets using computational chemistry. To make molecules computer-understandable, we use expert-derived "descriptors" and develop tools for generating them. Finally, we will look at computer-aided design of molecules and catalysts with target properties, for example reactivities.

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