Ab initio chemical reaction design and discovery through automated pathway exploration

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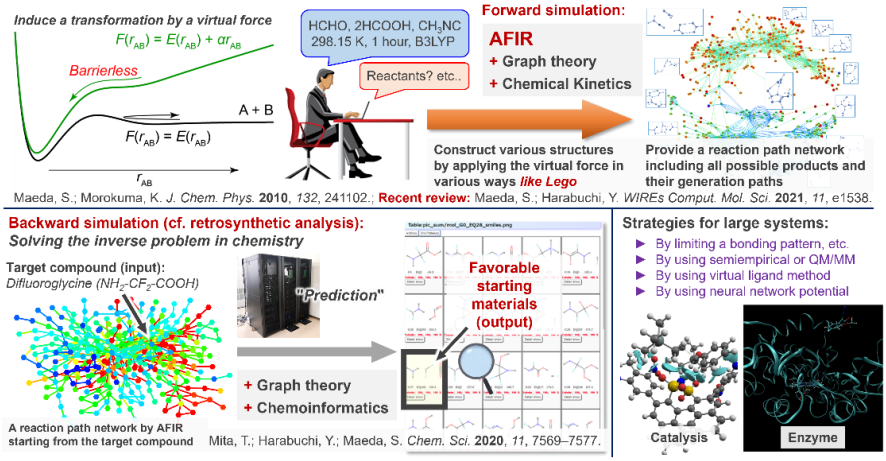
The motion of atoms during a chemical reaction, hereafter referred to as the reaction path, can in principle be elucidated by repeated quantum chemical calculations in all energetically feasible atomic configurations. However, the number of possible atomic arrangements involved in a reaction path can be enormous. Previous studies have therefore relied on assumptions, i.e., human input, about the atomic configurations along the reaction path under consideration. To address this problem, we have developed an automated reaction path search method called artificial force induced reaction (AFIR) [1]. AFIR automatically explores possible reaction paths by systematically inducing geometric transformations in a molecule using a virtual force, providing a network of reaction paths.

When AFIR is combined with a chemical kinetics method called rate constant matrix contraction (RCMC) [2], on-the-fly kinetic simulation can be performed [3]. Both forward and backward modes are available in on-the-fly kinetic simulations [3]. The forward mode starts the search from a given reactant and proceeds towards possible products. On the other hand, the backward mode starts the search from a given product towards possible reactants that give the product with high yields. Finally, the forward mode predicts all possible products along with their reaction yields and the backward mode predicts all possible reactants along with the yields of the input product in reactions from these reactants. In my talk, I will discuss the forward and backward on-the-fly kinetic simulations [3] shown in the scheme below, their applications to real-world reaction discovery [4], and more.



Bibliography:

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