Efficiently Charting Chemical Reaction Space with First-Principles Methods

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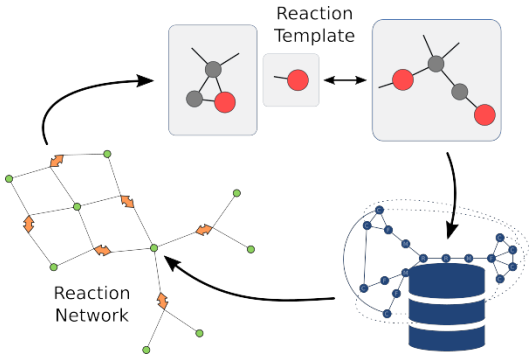
Much algorithm development has been devoted to the computer-based automated exploration of chemical reaction networks in recent years.[1] These reaction network-based methods aim to establish a sufficiently complete reaction network to allow for reliable predictions, detailed understanding, and, eventually, the design of chemical processes. A comprehensive reaction network consists of all thermodynamically and kinetically relevant intermediates (under reaction conditions) and all reaction paths that connect them. Due to conformational diversity, a reaction network generated for relatively simple chemical processes can be vast if it is complete. This poses a set of challenges for methodology and software.[2] Here, we will present the current developments of our mechanism exploration automaton, called Chemoton[3], in its latest release version[4,5] and new developments to accelerate explorations[6].



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