Modelling reactivity and selectivity in chemistry: from concept to reaction path

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Abstract

Rationalising and predicting chemical reactivity and selectivity is a central concern of theoretical chemistry. Several frameworks were proposed to address this, which can be roughly separated into two classes : the implicit approaches, where chemical properties are infered from some well-designed quantities (named descriptors) calculated on key reaction intermediates, and the explicit ones, where one unfolds complete reaction profiles and analyses reactivity and selectivity through the associated energetics.

In this presentation, I propose to show you on some examples studied in my group how such approaches can be put in action (sometimes jointly), allowing to refine our conceptualisation of chemical reactivity, but also ultimately granting us with the possibility to predict efficiently the outcome of chemical reactions.