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Automated Discovery of Reaction Mechanisms and Kinetics Using Dynamics Simulations

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A novel computational method is proposed in this talk for use in discovering reaction mechanisms and solving the kinetics in reactive systems [1,2]. The method does not rely on either chemical intuition or assumed a priori mechanisms, and it works in a fully automated fashion. It has two components: accelerated chemical dynamics simulations and a post-processing geometry-based algorithm that selects suitable transition state (TS) guess structures.
Two levels of electronic structure calculations are involved in the procedure: a low level (LL) is used to integrate the trajectories and to optimize the TSs, and a higher level (HL) is used to refine the structures.
Our method has been successfully employed in the study the dissociation channels of formaldehyde, formic acid (FA), vinyl cyanide (VC), propenal, acryloyl chloride (AC), and protonated uracil (uracil-H+), and also in the study the cobalt-catalyzed hydroformylation and hydrogenation of ethylene [3].
Figure 1 shows a flow-chart outlining the different steps of the automated method needed to study organometallic catalysis.

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