EXPLORING TRANSITION METAL CATALYZED REACTIONS VIA AB INITIO REACTION PATHWAYS

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The study and prediction of chemical reactivity is one of the most influential contributions of quantum chemistry. A central concept in the theoretical treatment of chemical reactions is the reaction pathway, which can be quite difficult to integrate accurately and efficiently. This talk will outline our developments in the integration of these pathways on ab initio potential energy surfaces. We will also describe results from recent studies on the kinetics of transition metal catalyzed reactions, including the importance of vibrational coupling to the reaction coordinate and the role of this coupling in catalytic rate enhancement.