

## **Predicting a chemical reaction, its products, yields, and mechanisms by exploring quantum chemical potential energy surfaces**

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In this talk, I will present a state-of-the-art computational method for predicting chemical reactions by exploring quantum chemical potential energy surfaces. The artificial force induced reaction method, in which a virtual force is applied to a given molecule or complex to induce structural changes, can automatically generate reaction path networks that exhaustively cover different reaction pathways. Combined with the rate constant matrix contraction method, which allows efficient and deterministic analysis of complex reaction path networks, on-the-fly kinetic simulation is realized, in which reaction paths are explored while solving the rate equations. On-the-fly kinetic simulation can automatically reveal a chemical reaction, its products, yields, and mechanisms. Its development, application to known and unknown reactions, and use in reaction design are discussed.