Theoretical exploration of astrochemical reactions: Leveraging ring-polymer molecular dynamics and machine-learning techniques

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We have embarked on the research project entitled “Next Generation Astrochemistry”. Our mission is to comprehend reaction mechanisms[1-7] and furnish reliable thermal rate coefficients to enhance the precision of the rate coefficients in the astrochemical database.

To understand chemical reactions, a potential energy surface spanning the 3*N*-6 dimensions, where *N* represents the number of atoms, is necessary. We have recently developed several full-dimensional potential energy surfaces (PESs) such as $H^- + C_2H_2 \rightarrow H_2 + C_2H^-$, $NH_3^+ H_2 \rightarrow NH_4^+ + H$, and $(HCOOH)H^+ \rightarrow CO + H_3O^+ / HCO^+ + H_2O$ reactions[1-3]. To develop these PESs, we employed a machine-learning technique, utilizing polynomial fitting from preliminary dynamics data and potential energies at various intrinsic reaction coordinates.[4]

In the cold environments typical of the interstellar medium, nuclear quantum effects can profoundly impact chemical dynamics. Hence, we employed the ring-polymer molecular dynamics (RPMD) simulation method. Our investigations have revealed that nuclear quantum effects and the quantum fluctuation of nuclei play a crucial role not only in the aforementioned collision reactions[1-3] but also in determining the H_2 sticking probability on ice clusters.[5]

In this presentation, we will introduce our recent research on the branching dynamics of $H_3^+ + C_2H_4 \rightarrow H_2 + C_2H_5^+ / 2H_2 + C_2H_3^+$ and $H_3^+ + HNCO \rightarrow H_2 + HNCOH^+ / H_2 + H_2NCO^+$ reactions. Additionally, we delve into the transition state dynamics of $CH_3OH + OH^\bullet \rightarrow CH_3O^\bullet + H_2O$ with the goal of comprehending the intricate reaction mechanism post-transition state from a dynamical viewpoint, a perspective unattainable through the statistical transition state theory.

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