

NSFC Funded Project Made Significant Progress in Quantum Dynamics

Prof. Zhang Donghui, Prof. Yang Xueming and colleagues in Dalian Institute of Chemical Physics, CAS published on *Science* in July, 2011 an article “Experimental and Theoretical Differential Cross Sections for a Four-atom Reaction: $\text{HD} + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{D}$ ”, summarizing results of a research project funded by NSFC. This is a significant progress made by Chinese scientists in chemical reaction dynamics.

Differential cross sections (DCSs) of chemical reactions characterize the effective target area of the colliding reactants that leads to the scattering of reaction products into a particular angle range. They are the most detailed observables that can be measured experimentally, and also one of the most important physical quantities in chemical reactions. To obtain DCSs theoretically, one needs to solve Schrödinger equations for nuclear motions on a given potential energy surface. In 1976, Schatz of California Institute of Technology and his mentor Kuppermann first converged calculations of state-to-state DCSs for the $\text{H} + \text{H}_2$ reaction, ushering in a new era for accurate calculations for three-atom reactions. In the following thirty years, with the development of more effective quantum scattering methodologies and modern computer technology, researches on three-atom state-to-state quantum dynamics have achieved great progress. Given an accurate potential energy surface for an atom-diatom reaction, quantum scattering theory is now able to provide dynamical quantities that compete in accuracy with state-of-the-art experiments. Close interaction between theory and experiment on three-atom reactions has further clarified many underlying mechanisms. However, extending the success of calculations for three-atom reactions to four-atom reactions is not a trivial task. The number of degrees of freedom increases from three for a three-atom system to six for a four-atom system, which tremendously increases in calculation difficulty and complexity. For this reason, no great progress has been made in the past thirty years for the accurate calculations of four-atom reactions.

With long-term effort, Prof. Zhang and his team developed an effective calculation method and theory for four-atom state-to-state reactions, which provided a possible approach to full-dimensional state-to-state quantum dynamics. With the help of Prof. Xu Xin from Fudan University, the team developed a more accurate energy surface for OH_3 system, and obtained the full-dimensional quantum DCS for $\text{HD} + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{D}$ reaction in excellent agreement with those from a high-resolution, crossed-molecular beam experiment by Prof. Yang Xueming’s team. The $\text{H}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{H}$ reaction is the easiest four-atom reaction and plays an important role in combustion chemistry. Since it involves three hydrogen atoms, it is an ideal model for accurate quantum dynamics and a benchmark reaction for four-atom reactions. As its isotopic variant, the $\text{HD} + \text{OH}$ reaction has significant meaning for the study of four-atom reactions.