Exploring Gas-Surface Reaction Dynamics with Neural Network High-Dimensional Potential Energy Surfaces

SPEAKER: Bin Jiang, University of Science and Technology of China
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VENUE: Room 264, Geography Building, Zhongbei Campus, ECNU
HOST: Xiao He, East China Normal University

ABSTRACT OF THE TALK
Gas-surface reactions play an important role in many heterogeneous catalysis processes such as methane steam reformation and water-gas shift reactions. An in-depth understanding of these dynamical processes is of great importance and requires a completely dynamical model. However, most of previous theoretical studies have neglected the degrees of freedom of the surface atoms, i.e., within the static surface approximation. In this regard, we recently studied the unprecedented vibrational mode specificity of methanol on Cu(111). Moreover, we have developed high-dimensional potential energy surfaces (PESs) including surface atoms for describing the molecule-surface energy exchange, taking advantage of the Behler-Parrinello type of neural network (NN) method. Taking HCl/Au(111) and CO2/Ni(100) systems as examples, we show that molecular dynamics simulations on NN PES reproduce well the much more expensive on-the-fly ab-initio molecular dynamics (AIMD) results with much better statistics. More importantly, we can obtain a dynamically converged high-dimensional PES with as few as one hundred AIMP trajectories, which enable us to predict more demanding state-to-state scattering properties of polyatomic molecules on metal surfaces.

BIOGRAPHY
Professor Bin Jiang received his B.S. and Ph.D. degrees at the Nanjing University in 2007 and 2012, respectively. After that he worked as a postdoctoral researcher at the University of New Mexico. In 2015, he joined Department of Chemical Physics at University of Science and Technology of China. He has been focusing on the theoretical studies of the chemical reaction dynamics, which mainly involve elementary chemical reactions of small molecules in gas phase and on metal surfaces. Especially, he has developed efficient computational tools for constructing high-dimensional potential energy surfaces and performing quantum dynamics calculations of gas-surface reactions. He has published more than 90 peer-reviewed papers including those on Science, PNAS, J. Am. Chem. Soc, Angew. Chem. Int. Ed., Phys. Rev. Lett., Chem. Sci., J. Phys. Chem. Lett., etc., which have been cited by more than 2800 times (H-index=31). He has delivered several invited talks at internationally established conferences such as Gordon Research Conference and Stereodynamics conference.