# 北京大学量子材料科学中心

## International Center for Quantum Materials, PKU

## Special Seminar

# Nonadiabatic molecular dynamics investigations on the ultrafast charge dynamics at Interfaces


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**Time: 2:00pm, July 19, 2016 (Tuesday)**

**时间：2016年7月19日 （周二）下午2:00**

**Venue: Room W563, Physics building, Peking University**

**地点：北京大学物理楼，西楼563**

## Abstract


The ultrafast dynamics of photo-excited charge carriers plays an important in optoelectronics and solar energy conversion. Using nonadiabatic molecular dynamics simulation, we study the ultrafast charge dynamics at $CH_3OH/TiO_2$ and $MoS_2/WS_2$ interfaces. For $CH_3OH$, we study the forward and backward hole transfer between $TiO_2$ and $CH_3OH$ as well as the whole hole relaxation process to valance band maximum (VBM). First, we found that the hole trapping ability of $CH_3OH$ depends on the adsorption structure strongly. Only when the $CH_3OH$ is deprotonated to form chemisorbed $CH_3O$, there will be ~15% hole trapped by the molecule. Second, we found the time scales of forward hole transfer process from $TiO_2$ to $CH_3O$ (hole trapping process) and hole relaxation to VBM strongly depend on the temperature. When the temperature decreases from 300K to 30K, for hole trapping process, the time scale increases from 150 fs to ps magnitude. The hole relaxation process to VBM is also slow down significantly. This can be interpreted by the reduction of the non-adiabatic coupling and the phonon occupation. Our studies provide valuable insights into the photogenerated charge dynamics near molecule/$TiO_2$ interface.

For $MoS_2/WS_2$, we show that instead of direct tunneling, the ultrafast interlayer hole transfer is strongly promoted by an adiabatic mechanism through phonon excitation. At room temperature the interlayer charge transfer in $MoS_2/WS_2$ is ultrafast with a timescale of 20 fs which is in good agreement with the experiment. This ultrafast hole transfer process can be suppressed by decreasing the temperature to 100K, which reduces the phonon occupation and the charge transfer is then dominated by direct tunneling, which happens at the time scale longer than 300 fs. The atomic level picture of phonon-assisted ultrafast mechanism revealed in our study is valuable both for the fundamental understanding of ultrafast charge carrier dynamics at vdW hetero-interfaces as well as for the design of novel quasi-2D devices for optoelectronic and photovoltaic applications.


## About the speaker

赵瑾，1998 年7 月毕业于中国科学技术大学物理系，并在2003 年12 月于中国科学技术大学理化科学中心（现并入合肥微尺度国家实验室）获得博士学位（指导教师：侯建国院士，杨金龙教授），博士论文获中科院优秀博士论文奖。2004 年3 月起在美国匹兹堡大学Hrvoje Petek 教授组内工作，研究各种表面界面的电子结构及动力学性质，负责组内所有理论计算工作。2008 年8 月起成为匹兹堡大学物理系研究助理教授，2010 年初成为中国科学技术大学物理系及合肥微尺度国家实验室教授，匹兹堡大学兼职教授（adjunct Prof.），并入选百人计划。2013年获基金委优秀青年基金资助。研究涉及到几个方向：1.激发态载流子动力学研究；2. 基于低维材料的纳米器件研究；3.表面光催化机理研究等。