



## Seminar

# Non-Adiabatic Molecular Dynamics Investigations on the Excited Carrier Dynamics

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**Time: 10:00am, May. 8, 2018 (Tuesday)**

**时间: 2018年5月8日 (周二) 上午 10:00**

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

**地点: 北京大学物理楼 西563**

### Abstract

The ultrafast dynamics of photo-excited charge carriers in condensed matter systems plays an important role in optoelectronics and solar energy conversion. Yet it is challenging to understand the multi-dimensional dynamics in time, energy, real and momentum spaces at the atomic scale. Combining the real-time time-dependent Density Functional Theory (TDDFT) with fewest surface hopping scheme, we use homemade time-dependent *ab initio* nonadiabatic molecular dynamics code (Hefei-NAMD) to simulate the excited carrier dynamics in different condensed matter systems including two-dimensional vdW heterostructures and molecule/metal oxide interfaces. The time-dependent dynamics of excited carriers are studied in energy, real and momentum spaces. In addition, the coupling of the excited carriers with phonons, polarons, defects and molecular adsorptions are investigated. Recently, by combining with path-integral techniques, the nuclear quantum effects have been included in the NAMD simulations. Our state of art NAMD studies provide an atomic insight into the ultrafast dynamics of the excited carriers in condensed matter systems.

### About the Speaker

赵瑾, 1998年毕业于中国科学技术大学物理系, 2003年于中国科学技术大学理化科学中心获得博士学位(指导教师: 侯建国院士, 杨金龙教授)。2004年3月起在美国匹兹堡大学HrvojePetek教授组内工作。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。赵瑾教授的研究小组关注于利用第一性原理计算从时间、空间、动量与能量等多个尺度对激发态动力学的超快过程进行描述, 同时研究激发态载流子与声子、极化子、缺陷、边界等的相互作用。迄今为止赵瑾教授共发表SCI论文76篇, 包括3篇Science, 1篇Nature Photonics, 5篇Phys. Rev. Lett., 2篇Chem. Rev., 1篇Acc. Chem. Res., 1篇Annu. Rev. Phys. Chem., 6篇J. Am. Chem. Soc., 4篇Nano Lett., 7篇ACS NANO, 2篇Nature Communications, 16篇Phys. Rev. B等。