

# 凝聚态物理-北京大学论坛

<http://www.phy.pku.edu.cn/~icmp/forum/2015/2015chun.xml>

## Excited state electron-ion dynamics at interface

孟胜 研究员

**Abstract:** Real-time time-dependent density functional theory (TDDFT) has been implemented using local atomic basis, which enables large scale simulations on electron-ion dynamics at more realistic complex interface systems. The electron-ion evolution is driven by a Hamiltonian that build upon excited state electron density. This allows us to demonstrate the working principles of hybrid solar cells especially that involving charge separation and collection dynamics purely based on quantum mechanics. The method also yields precise prediction of the timescale for ultrafast electron injection from chromophores to semiconductors, in response to various interface structural details (molecular size, anchor group, binding mode, defects) and environment (excitation level, solvents). Consequently we could build a “virtual solar cell” producing macroscopic current-voltage relationships with only input being molecular composition. The methods are also used for investigating ultrafast electron transfer in dichalcogenides heterostructures, solvated electrons supported on surfaces, and plasmonic water splitting.

**About speaker:** Dr. Sheng Meng is a professor of surface physics at Institute of Physics (IOP), Chinese Academy of Sciences since 2009. He obtained his Bachelor degree in physics from University of Science and Technology of China (USTC) in 2000, and Ph.D. degree from IOP/Chalmers University of Technology, Sweden in 2004. During 2005-2009, he worked at Harvard University's Department of Physics first as a post-doctoral researcher then a research associate.

Dr. Meng's research interests focus on quantum interaction and excited state quantum dynamics at materials surface. His previous work started with simple and mysterious molecule: water. Current interests include ambient quantum materials, DNA-nanotube interaction, and energy conversion mechanisms in artificial photosynthesis. He has published ~80 technical papers in peer-reviewed journals, and has received 2600+ citations.

**时间：6月4日（星期四）15:00—16:30**

**地点：北京大学物理大楼中212教室**

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