Seminar

Non-Adiabatic Molecular Dynamics Investigations on the Excited Carrier Dynamics

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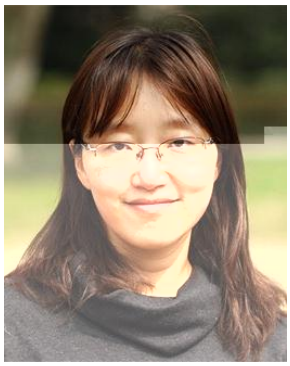

Time: 10:00am, May. 8, 2018 (Tuesday)

: 2018 5 8 10:00

Venue: Room W563, Physics Building, Peking University

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

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