

## Excited electron-phonon coupling

**Abstract** Real-time time-dependent density functional theory (RT-TDDFT) using local kinetic basis sets enables large-scale simulation of electron-phonon coupling in finite systems. The electron-phonon event is simulated up to excited state electron density. This allows us to determine the electron-phonon scattering rates involving charge separation and electron-phonon coupling in quantum mechanical method also yields precise phonon dispersion relation in carbon nanotubes, nanowires, and semiconductors. The structural changes of carbon nanotubes, nanowires, and semiconductors (excitation level, solvation) are investigated. Consequently, we could build microscopic current-voltage relationships with only input parameters. The methods are also applied for investigating electron-phonon coupling in carbon nanotubes, nanowires, solvated electrons supported on carbon nanotubes, and carbon nanowires.

**About speaker** Dr. Sheng Meng is a professor of surface physics at the Chinese Academy of Sciences since 2009. He obtained his Bachelor's degree from the University of Science and Technology of China (USTC) in 2000, and his Master's degree from the University of Science and Technology of China (USTC) in 2003. During 2005-2009, he worked at the Department of Physics, Chalmers University of Technology, Sweden. During 2010-2014, he worked at the Department of Physics, Chalmers University of Technology, Sweden. His research interests are in the field of surface physics, particularly in the area of electron-phonon coupling, electron transport, and surface catalysis. He has published over 100 papers in international journals and has been involved in several international collaborations. He is currently a member of the Chinese Academy of Sciences and the Chinese Academy of Engineering.

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