北京大学量子材料科学中心

International Center for Quantum Materials, PKU

Seminar

Multi-phonon processes in solids from first-principles

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Time: 10: 00 am, May. 28, 2019 (Tuesday)

时间：2019年5月28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会议室

Abstract

Hot carrier capture by defects in semiconductors and resonant Raman scattering are both shown to be multi-phonon processes. We have constructed a comprehensive computational approach for these processes using the density functional theory. For carrier capture, we distinguish between thermal equilibrium and nonequilibrium conditions. In the thermal-equilibrium case, capture is mediated by a nonadiabatic perturbation Hamiltonian, which is equal to linear electron-phonon coupling to first order. In the nonequilibrium case, the primary capture mechanism is within the Born-Oppenheimer approximation (adiabatic transitions), with coupling to the defect potential inducing Franck-Condon electronic transitions, followed by multi-phonon dissipation of the transition energy, while the nonadiabatic terms are of secondary importance. We report first-principles density-functional-theory calculations of the capture cross section for a carbon defect in GaN. As a second example, we present a first-principles calculation of the resonant Raman spectrum of MoS_2/WS_2 heterostructure. In this case, atomic displacements between the electronic ground state and the excited states due to charge transfer between the two layers lead to finite phonon matrix elements allowing inelastic multi-phonon relaxation to accompany the absorption and emission of photons. For each excited state, the relative Raman intensity, peak width and shape are obtained directly from a sum over all configurations of multiple phonon modes and compared to experiments. Temperature dependence of the Raman peak is calculated, which also agrees well with experiment, and predicted resonance intensity as a function of laser energy is calculated.

About the speaker

Prof. Xiaoguang Zhang obtained his B.S. in Physics at Peking University in 1983, and received his Ph.D. in Physics from Northwestern University in1989. His main research interests focus on:

1. Theory and modeling of electron transport in magnetic tunnel junctions, molecular junctions, polymers and nanoscale materials.
2. Calculation of electron mobility and defect capture cross section in semiconductors.
3. Image informatics for scanning tunneling potentiometry.