北京大学量子材料科学中心

Seminar

Multi-phonon processes in solids from first-principles

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

2019 5 28 10:00

Venue: Room W563, Physics building, Peking University

563

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 fin6Tm0BM rem0g0G[( )]TJETQ05.2 817 8 r