MAR12-2011-005186

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Phonon-assisted Auger recombination and optical absorption in semiconductors

EMMANOUIL KIOUPAKIS, University of Michigan

The coupling of charge carriers to lattice vibrations is an important process in materials that enables higher-order electronic transitions. We employed first-principles methods based on density functional theory to study various phonon-assisted electronic processes in semiconductors, such as Auger recombination and optical absorption. Auger recombination is a three-particle non-radiative recombination process that affects optoelectronic devices at high carrier densities. Phonon-assisted Auger recombination, in particular, is expected to be important in wide-band-gap materials. We describe the computational formalism to study phonon-assisted Auger recombination in semiconductors. We show that these indirect Auger processes are strong in the group-III nitrides and affect the high-power performance of visible light-emitting diodes. Moreover, the electron-phonon interaction facilitates the absorption of light by free carriers in doped semiconductors and transparent conducting oxides, which limits the output power of optoelectronic devices. We describe how first-principles techniques can be used to calculate the phonon-assisted free-carrier absorption coefficient in semiconductors and discuss our results for the group-III nitrides. In addition, the electron-phonon coupling enables indirect interband optical transitions in indirect-gap materials such as silicon. These processes are instrumental for the absorption of visible light and the operation of silicon solar cells. We present our first-principles formalism and calculated results for the phonon-assisted absorption of visible light in silicon. Our calculated results are in very good agreement with experiment. Our work highlights the significance of first-principles methods in understanding key microscopic quantum phenomena in technologically important materials and devices. Work done in collaboration with C. G. Van de Walle, P. Rinke, K. Delaney, A. Schleife, F. Bechstedt, D. Steiauf, H. Peelaers, J. Noffsinger, S. G. Louie, and M. L. Cohen. Support was provided by CEEM, SSLEC, NERSC, and Teragrid.