

MAR14-2013-006534

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

First principle prediction of shallow defect level binding energies and deep level nonradiative recombination rates¹
LINWANG WANG, Lawrence Berkeley National Laboratory

Accurate calculation of defect level energies in semiconductors and their carrier capturing rate is an important issue in ab initio prediction of semiconductor properties. In this talk, I will present our result work in ab initio shallow level calculation [1] and deep level caused nonradiative recombination rate calculation [2]. In the shallow acceptor level calculation, a large system up to 64,000 atoms needs to be used to properly describe the weakly bounded hole wave functions. The single particle Hamiltonian of that system is patched from bulk potential and central potential. Furthermore, GW calculation is used to correct the one site potential of the impurity atom. The resulting binding energy agrees excellently with the experiments within 10 meV. To calculate the nonradiative decay rate, the electron-phonon coupling constants in the defect system are calculated all at once using a new variational algorithm. Multiphonon process formalism is used to calculate the nonradiative decay rate. It is found that the transition is induced by the electron and the optical phonon coupling, but the energy conservation is mostly satisfied by the acoustic phonons. The new algorithm allows fast calculation of such nonradiative decay rate for any defect levels, as well as other multiphonon processes in nanostructures.

[1] G. Zhang, A. Canning, N. Gronbech-Jensen, S. Derenzo, L.W. Wang, "Shallow impurity level calculations in semiconductors using ab initio method," Phys. Rev. Lett 110, 166404 (2013).

[2] L. Shi, L.W. Wang, "Ab initio calculations of deep level carrier nonradiative recombination rates in bulk semiconductors," Phys. Rev. Lett. 109, 245501 (2012).

¹This work was supported by the Director, Office of Science (SC), Basic Energy Science (BES)/Materials Science and Engineering Division (MSED) of the U.S. Department of Energy (DOE) under the contract No. DE-AC02-05CH11231.