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Radiative and nonradiative recombination at defects in semiconductors[1]

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This talk will provide an overview of our recent work on the first-principles description of electron-phonon interactions at defects in semiconductors. Two aspects of this interaction have been addressed: (i) vibrational structure of defect luminescence bands [Phys. Rev. Lett. 109, 267401 (2012); New. J. Phys. 16, 073026 (2014)] and (ii) nonradiative carrier capture by means of multiphonon emission [Phys. Rev. B 90, 075202 (2014)]. The first process is related to the diagonal part, while the second one is related to the off-diagonal part of electron-phonon coupling. We show that in many situations it is necessary to go beyond traditional semilocal approximations to density functional theory not only to obtain a reliable description of defect geometries and charge-state transition levels, but also to accurately account for the interaction with the lattice during radiative or nonradiative processes. In particular, we demonstrate that hybrid density functionals yield luminescence lineshapes and nonradiative capture rates in very good agreement with experiment. Work performed in collaboration with Q. Yan, C. E. Dreyer, J. L. Lyons, and C. G. Van de Walle.

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