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Ab initio calculations of non-radiative carrier trapping due to deep impurity levels¹ LIN-WANG WANG, Lawrence Berkeley National Laboratory, LIN SHI, Suzhou Institute of Nano-Tech and Nano-Bionics, CAS — Non-radiative carrier decay due to deep impurity levels in semiconductors is an important process which affects the efficiencies of devices from solar cells to light emitting diode. This process is due to multiple phonon emission. Despite of the fact the analytical formalisms have been derived long time ago, so far there is no direct ab initio calculations due to the high cost of calculating all the electron-phonon coupling constants. Here we introduce an algorithm which calculates all the electron-phonon coupling constants at once, hence allows the ab initio calculations of such processes. Another approximation is introduced to calculate the phonon modes of a given impurity system. We use a $Zn_{Ga}-V_N$ paired defect in GaN as an example to study this process. We found that while most of the promoting phonon modes (used to promote the transition with the electron-phonon coupling) come from the optical modes, the accepting phonon modes (used to satisfy the energy conservation) come mostly from the acoustic phonons.

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