Accurate and effective computation of the multi-phonon nonradiative transition

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Received April 7, 2020; accepted April 24, 2020; published online May 19, 2020

Citation: S.-H. Wei, Accurate and effective computation of the multi-phonon nonradiative transition, *Sci. China-Phys. Mech. Astron.* **63**, 117331 (2020), <https://doi.org/10.1007/s11433-020-1570-y>

Nonradiative carrier recombination at a defect or impurity level can reduce the collection of photo-generated carriers and suppress luminescence. Therefore, understanding the underlying mechanism and providing an accurate theoretical prediction of the carrier capture rate (CCR) of a defect in a semiconductor are important for both semiconductor physics and device engineering [1–5]. The *ab initio* calculation of the CCR is time-consuming because it requires an accurate calculation of the defect-induced electron-phonon coupling matrix in a large supercell containing a single point defect. It becomes possible only recently after Wang’s group [3] developed an effective method to calculate the defect-induced electron-phonon coupling matrix [3–5]. However, almost all current approaches are based on the assumption that the phonon modes before and after the electronic transition are the same; while in reality, for the defects with different charge states before and after the transition, their phonon modes could be quite different, especially for the localized deep-level defects that often involve large local distortions associated with the charge state of the defect [5]. Therefore, it is crucial to investigate how the so-called anharmonic effect affects the calculation of the CCR.

In this paper entitled “Anharmonic multi-phonon non-radiative transition: An *ab initio* calculation approach” [1], the authors provide an analysis of Huang’s original non-

radiative multi-phonon (NMP) theory and demonstrate that it provides an analytical expression for the coupling constant in the widely used Marcus theory [3]. Most importantly, the previously ignored anharmonic effects are corrected by taking into account local phonon-mode variations for different charge states of a defect, and a detailed calculation procedure is provided. They show that after the correction, the calculated CCRs for the deep-level defects in prototype GaN and SiC are in better agreement with the experimental results.

Because the nonradiative carrier recombination plays a key role in understanding the semiconductor device physics [3–5], and the direct measurement of the CCR in experiment is still quite challenging, the accurate calculation of CCR becomes especially critical. This work has made a significant and timely contribution in this field [1]. This will certainly help us improve our understanding of the semiconductor defect physics and optoelectronic device performance.

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