Many body effects in the excitation spectrum of a defect in SiC

Michel Bockstedte[1,2], Andrea Marini[3], Oleg Pankratov[1] and A. Rubio[2]
[1]Nano-Bio Spectroscopy group and ETSF, Univerisdad del País Vasco UPV/EHU, Dpto. Fisica de Materiales, CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain,
[2]Lst. f. Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Erlangen, Germany
[3]ETSF, Dipartimento di Fisica, Universit di a Roma Tor Vergata, Roma, Italy

Defect excitations combine the many-body effects in both extended and localized states. The insertion of electrons into defect states invokes on-site correlation due to electron-electron repulsion expressed by the Hubbard U. Defect-to-band transitions involve two particles, the electron and the hole. To self-energy effects this adds excitonic correlation energy of yet unknown size. Density functional theory (DFT) provides insight into the physics of defects in covalent semiconductors in many cases, helping for instance the identification of vacancy-related defects in SiC [1]. Despite the success of this common approach, it has severe shortcomings: the description of the bonding of the bulk crystal may be insufficient within common approximations for exchange and correlation, like the local spin density approximation (LSDA), the position of defect levels in the band gap is affected by the well-known Kohn-Sham band gap error, and excitations cannot be assessed rigorously. Many-body perturbation theory allows to resolve these issues [2]. The quantitative prediction of absorption spectra of a wide-class of systems from insulators to surfaces, to nanotubes and polymers became tractable only recently by solving the Bethe-Salpeter equations (BSE) and accounting for the G_0W_0 self-energy. Application of this approach to the case of defects are scarse.

We investigated many-body effects in the excitation spectrum of the positive carbon vacancy in SiC. The identification of this prototypical defect as an electron paramagnetic resonance (EPR) center was established on the basis of the DFT-LSDA calculations [1]. In EPR experiments under illumination [3], excitation thresholds were assigned to the defect ionization levels with respect to the neutral defect. However, the interpretation of the spectra in terms of the thresholds for the quenching of the paramagnetic state and its re-ionization are in conflict with the DFT-LSDA values.

For this defect, we demonstrate the importance of correlation effects at the level of GW and BSE. Charge state-dependent corrections to DFT-LSDA affect the ionization levels (up to 0.5 eV) and the electron-electron repulsion U ($\sim$0.3 eV). The electron-hole attraction (Excitonic effects) introduces a sizeable red shift ($\sim$0.23 eV) of the spectra. We show that two ionization of the defect (into the doubly positive or neutral vacancy) are competing possibilities. More importantly, the calculated transition energy thresholds for the two channels indicate that the current interpretation of photo-EPR spectra based on the assumption of a photoionization via the neutral defect has to be corrected. For the range of photon energies in which photo-EPR experiment identified thresholds only the former ionization channel is active. This unambigously rectifies the earlier experimental assignment of transitions and the assessment of ionization levels.

[1] M. Bockstedte, M. Heid, and O. Pankratov, Phys. Rev. B 67, 193102 (2003). T. Umeda et al., Phys. Rev. Lett. 96, 145501 (2006); N. T. Son et al, Phys. Rev. Lett. 96, 055501 (2006).
[2] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. 74, 601 (2002).
[3] N. T. Son, B. Magnusson, and E. Janzen, Appl. Phys. Lett. 81, 3945 (2002); J. Dashdorj, M. E. Zvanut, and J. G. Harrison, J. Appl. Phys. 104, 113707 (2008).