Comparative Study of DFT and GW Approximation on the Germanium-Vacancy Center

E. Aylin Melan[1,2,3*], Thijs G. I. van Wijk[1,2], Luc Henrard[3], Danny E. P. Vanpoucke[1,2]

[1]*Hasselt University, Institute for Materials Research (imo-imomec), Quantum & Artificial intelligence design Of Materials (QuATOMs), Martelarenlaan 42, B-3500 Hasselt, Belgium*
[2]*imec, imo-imomec, Wetenschapspark 1, B-3590 Diepenbeek, Belgium*
[3]*University of Namur, Namur Institute of Structured Matter (NISM), Rue de Bruxelles 61, 5000 Namur, Belgium*
EsinAylin.Melan@UHasselt.be

Diamond color centers have a long history of scientific interest due to their unique properties that can be applied in high-tech fields such as single photon emitters and magnetic sensing. Although over 500 color centers have been identified, only a few are identified with an atomic scale structure[1,2]. Additionally, distortions of the color centers, such as strains that are often present in (nano)diamonds, can alter their optical properties, leading to even more defect possibilities in diamond[3].

This project aims to develop a method for accurately predicting diamond quasiparticle band structures using delta machine learning (ΔML) based on low-cost calculations, like a Density Functional Theory (DFT) calculation. To make efficient (sustainable) use of the generated training data, our current focus lies in studying the electronic structure of the germanium-vacancy (GeV) center using different first principles approaches. This study compares DFT calculations with the GW approximation for the neutral, positively, and negatively charged GeV centers. Here, the former approach is a widely used approximation in solid state research for its relatively cheap calculations that have results comparable to experiments. The GW approximation calculates the system's self-energy, which comes with more accurate models for the excited energy states, but it has a much higher computational cost. This study provides insight into the GeV center and as well forms the first set of data needed to build up a database directed at the ΔML of the electronic structures of the diamond defects.

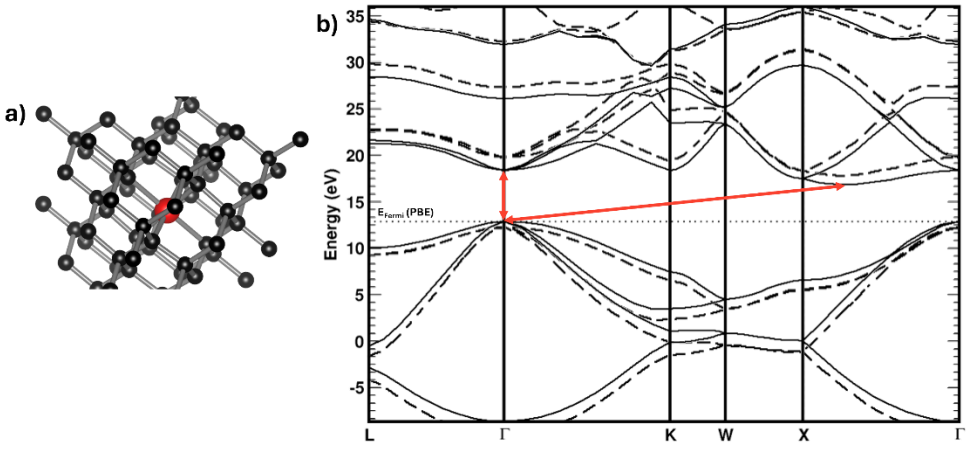

Figure 1 – a) Ball-and-stick representation of GeV in diamond b) Band structure of bulk diamond calculated using PBE (solid line) and single-shot GW (dashed line) method. The direct band gap is calculated to be 5.6 eV using PBE and 7.5 eV using GW, while the indirect band gap values are 4.1 eV for PBE and 5.7 eV for GW.

References

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