Straining color centers in diamond: DFA study of the GeV Zero-Phonon-Line.

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ABSTRACT

Color centers in diamond are of interest to a wide range of high-tech applications such as quantum information technology and nano-sensing.[1-3] In such practical applications, optical readout of the zero-phonon-line (ZPL) provides an direct means of gaining information on the color center state. In this work, we model the impact of strain and defect concentration on the ZPL position by means of Density Functional Approximations (DFA) to elucidate their experimental observation in nanocrystalline diamond films.

We have modelled the GeV-color center for concentrations ranging from 0.1% to 1.5% using DFA calculations (GGA and hybrid level). At each concentration, the super cells were strained both isotropic and anisotropic to mimic the possible experimental conditions experienced in nanocrystalline films. For three charge states (GeV^0, GeV^+ and GeV^-), the electronic structure was investigated in terms of the local charge distribution (Hirshfeld-I atoms-in-molecules method [4]) and ZPL position.

Although DFA provides an efficient quantum mechanical modeling tool, the cost for studying large systems with high accuracy can still be formidable. Our case study above, therefor also provides an excellent subject to quantify the impact of the functional and Brillouin zone sampling on the ZPL position. We show the consideration of an extended Brillouinzone not to be negligible for the ZPL, even in case of large super cells, and look for suitable approximations that could reduce the computational cost.

The results of our study provide a clear picture of the relationship between the ZPL-position and lattice strain, which is essential for understanding the behavior under experimental conditions in nano-crystalline diamond thin films, as well as insights in the model quality for DFA calculated defect properties.

References

[1] Damle, V. *et al.*, *Carbon* **2020**, 162, 1-12
[2] Vanpoucke, D.E.P. *et al. Diam. Relat. Mater.* **2019,** 94, 233-241
[3] Boldyrev, K.N. *et al. Diam. Relat. Mater.* **2022,** 126, 109049
[4] Vanpoucke, D.E.P. *et al. J. Comput. Chem.* **2013** 34(5), 405-417