Straining group-IV color centers in diamond: Using density functional theory to model the Zero-Phonon-Line shift

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Since the dawn of time, color centers in diamond have attracted great interest. Where initial interest focused on gemstone quality, recent years saw a growing interest in their application for quantum information technology and nano-sensing.[1] For the latter, group-IV color centers gained interest due to their excellent Debeye-Waller factor, making them suitable for optically based quantum applications.[2]

In this work, we present a Density Functional Theory (DFT) study of the group-IV color centers in diamond. We investigate the impact of strain and defect concentration on the zero-phonon-line (ZPL), and use our theoretical results to shed light on the experimental observation of these ZPL in nanocrystalline diamond (NCD) films.

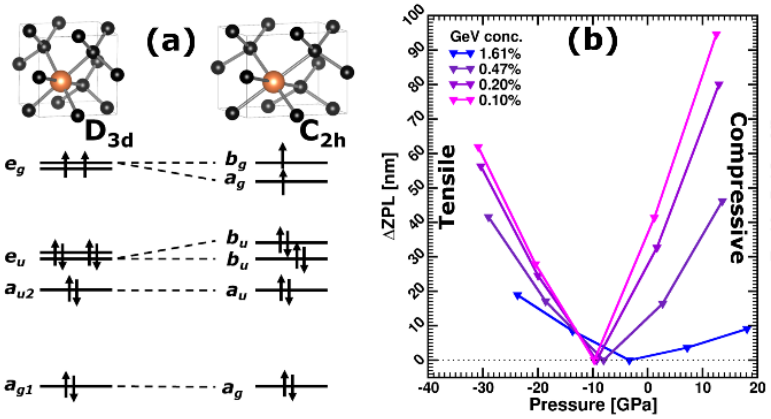

Figure 1: (a) GeV^0 level-splitting under linear strain, and (b) calculated resulting ZPL shift.

Although the atomic configuration of these centers is well established as a split-vacancy geometry, the impact of strain and concentration is less clear. Neutral and negatively charged color centers with concentrations of 1.5% down to 0.1% (64-to 1000-atom conventional cells) are modeled using DFT.[3] The supercells are strained both isotropic and anisotropic to mimic possible conditions in reality experienced in the NCD films. The evolution of the color center related bands is traced as function of strain, while the impact of concentration on the ZPL-shift is established.[3] The resulting ZPL-shift versus strain relationships are used to interpret the experimentally observed distribution of ZPL lines for the GeV and SnV systems. In the case of the GeV center, both blue-and red-shifted ZPL are explained, as well as the asymmetry in the experimentally observed ZPL distribution.[3]

[1] V. Damle, *et al* 2020 *Carbon* **162** 1-12
[2] E.Y. Guillaume, *et al* 2025 in *Nanophotonics with Diamond and Silicon Carbide for Quantum Technologies* **Chap. 5** ISBN: 978-0-443-13717-4
[3] T.G.I. van Wijk, *et al* 2025 *Carbon* **234** 119928