Title:

Modeling the impact of strain on Group-IV color centers in diamond: A first principles study of the ZPL position.

Abstract [300 words]

Color centers in diamond have a long history of interest, evolving from the quality of a prized gemstone to current day high-tech applications such as quantum information technology and nano-sensing.[1] Over time, hundreds of color centers have experimentally been identified, however, only few have been fully and decisively structurally characterized.[2] For high-tech applications, the group-IV color centers have gained interest in recent years due to their excellent Debye-Waller factor, making them suitable for optically based quantum applications.

In this work, we present a quantum mechanical study of the group-IV color centers in diamond. We investigate the impact of strain and defect concentration on the ZPL as these will help to elucidate the experimental observation of these ZPL in nanocrystalline diamond (NDC) films.

Although the structure of these centers is well established (split-vacancy), the impact of strain and concentration is less clear. Color centers with concentrations of 1.5% down to 0.1% (64-1000 atom conventional cells) were modeled using Density Functional Theory using hybrid functionals.[3] At different concentrations the supercells are strained both isotropic and anisotropic to mimic the possible conditions in reality experienced in NDC films. The evolution of the color center related bands is traced as function of the strain, and ZPL and defect formation energy were determined for neutral and charged color centers. Combining all these results provides a clear picture of the relationship between the ZPL-position and lattice strain, which is essential for understanding the behavior under experimental conditions in NDC thin films. These results are then used to elucidate the experimentally observed distributions of ZPL lines for GeV and SnV systems.[3]

[1] V. Damle, *et al*., *Carbon* **162**, 1-12 (2020),
[2] D.E.P. Vanpoucke, *et al. Diam. Relat. Mater.* **94**, 233-241 (2019).
[3] T.G.I. van Wijk, *et al.*, Carbon **234**, 119928 (2025)

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☐ Author Approval*

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Category:

Theory and Computational modelling of carbon materials

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- Density Functional Theory
- Zero-Phonon Line
- Diamond
- Strain