

Impact of strain on GeV color centers in diamond using *ab initio* calculations.

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Diamond color centers are considered excellent candidates for applications in quantum information processing, biosensors, and magnetometry. The interest in the GeV center arises mainly from its intense zero-phonon line and small phonon sideband. [1, 2, 3] Further research is needed to characterize the GeV center under experimental conditions. For this purpose, *ab initio* calculations provide valuable insights into the electronic energy levels of the color center under varying conditions such as strain and color center concentration. Additionally, group theory plays a very important role in the theoretical prediction of electronic energy levels. In this work, we aim to elucidate the effect of strain on the zero-phonon line (ZPL) by combining *ab initio* calculations and group theory.

The GeV color center is modelled using Density Functional Theory (DFT). To replicate different experimental conditions, different concentrations are modelled, using different sizes of supercells, ranging from 1.5% ($2 \times 2 \times 2$ conventional supercell) down to 0.1% ($5 \times 5 \times 5$ conventional supercell), an example of such a supercell is shown in 1 a). To draw solid comparisons between our results and either as-grown or implanted color centers, the structure relaxations were performed differently. For the first scenario, we varied the cell volume and shape, while for the second, we kept a constant set of lattice vectors.

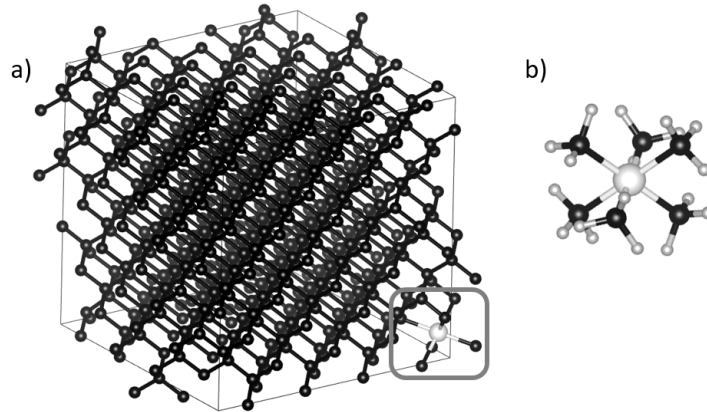


Figure 1: The GeV center depicted within (a) a $4 \times 4 \times 4$ supercell and (b) a $\text{GeC}_6\text{H}_{18}$ cluster, with Ge atoms represented in white, C atoms in black, and H atoms in grey.

After the initial relaxation of the structure, a static calculation is performed to find the electronic structure of the defect. The effect of an experimental strain can be replicated by stretching the relaxed structure hydrostatically or along a specific crystallographic orientation, changing the geometry and symmetry of the structure. The static calculations are performed with both a standard exchange-correlation functional (PBE) and a hybrid functional (HSE).

The calculated relaxed structure shows the expected D_{3d} symmetry. This symmetry is maintained after the structure was strained hydrostatically, but changes to C_{2v} for strain along the $\langle 100 \rangle$ direction. This can also be observed in the calculated energy levels, where some of the degeneracies, observed in the unstrained calculations with D_{3d} symmetry, are broken by the change to C_{2v} symmetry. Another observation is that the ZPL changes when strain is applied, both for the hydrostatic and $\langle 100 \rangle$ strain. To elucidate the identification of the color center energy levels within the diamond host lattice, DFT calculations are performed on a $\text{GeC}_6\text{H}_{18}$ cluster. Here, the defect atoms are placed in the same configuration as they would have in diamond, and each C atom is passivated with H atoms, as is shown in 1 b). This approach allows us to apply group theory directly to the energy levels of the GeV center and subsequently helps us to identify them in the diamond calculations.

References

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