Calculating the vibrational spectrum of the GeV defect in Diamond.

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As quantum information science advances, the demand for novel devices and materials capable of manifesting quantum effects becomes increasingly important. Diamond color centers are considered excellent candidates as single photon emitters. The interest in the GeV center and other group-IV color centers arises mainly from their intense zero-phonon line and small phonon sideband. [1,2] However, further research is needed to characterize the GeV center under experimental conditions, such as strain, which commonly arises during diamond growth and is known to alter the ZPL wavelength significantly. [3] To better understand these influences, a thorough examination of the phonon sideband is needed to characterise defects and zero-phonon line (ZPL) properties. Density Functional Theory (DFT) calculations provide valuable insights into the vibrational structure of the color center and serve as a powerful complement to experimental studies. [4,5] However, achieving precise vibrational calculations requires tremendous computational resources, often beyond what is available.

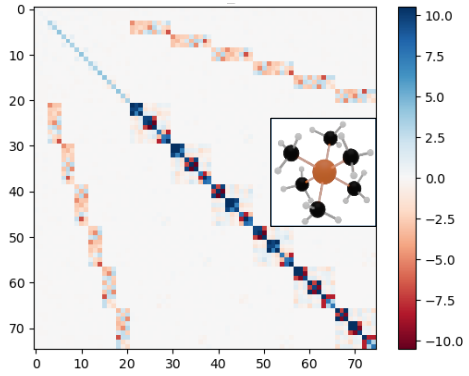

Figure 1: Dynamical matrix of GeC_6H_{18} cluster

In this work, we aim to predict vibrational spectra with Density Functional Theory (DFT) enhanced Machine Learning (ML). By combining these methodologies, we aim to address the critical need for accurate vibrational calculations in a computationally efficient manner. Before calculating the vibrational spectra of large supercells, this work focusses on GeC_6H_{18} and $GeC_{24}H_{42}$ clusters. These clusters represent the local region of the GeV center and have the same D_{3d} point group. A statistical analysis is performed on the dynamical matrix of these structures. The effect of local strain was replicated by stretching the structure hydrostatically or along a lattice vector, thereby changing the geometry and symmetry of the defect. This way a small dataset of dynamical matrices could be constructed to train a linear regression ML model. This basic machine learning model allows for predicting dynamical matrices of clusters with an arbitrary strain, leading to fundamental insights into the vibrational spectra of these color centers under experimental conditions.

References

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