DFT modeling of strained group-IV color centers in diamond

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Diamond color centers are considered as viable candidates for solid state qubits and single photon sources for quantum technological applications ranging from quantum sensing to quantum information processing [1]. Color centers are created through ion beam implantation or incorporation during chemical vapor deposition. This way most elements of the periodic table have been considered at some point in the past, even lanthanides like Eu, due to their sharp spectral properties [2]. However, in recent years, group-IV color centers have been gaining attention due to their excellent Debye–Waller factor, making them very suitable for optically based quantum applications. In such applications, a sharp and robust zero-phonon line (ZPL) are prime qualities sought after. Unfortunately, practical diamond based devices contain several sources of strain, originating from the ion beam implantation and annealing during device fabrication. This strain results in a shifting of the ZPL depending on the type of strain and magnitude experienced by the color center [3,4,5].

Using density functional theory (DFT) calculations, the impact of isotropic and anisotropic strain on the GeV and SnV centers in diamond is investigated, with the aim of understanding the experimentally observed distributions of ZPL positions. By using defect concentrations of 1.5% down to 0.1% (64–1000 atom conventional cells) we show that it is possible to extrapolate to experimentally relevant concentrations [3,4,5]. The calculated ZPL position and strain-induced shifts are presented for both neutral and negatively charged color centers. For the GeV^0 color center, both red and blue shifts are obtained for isotropic strain, while anisotropic strain only gives rise to a redshift. In case of the latter, the absolute magnitude of the shift is also significantly larger [3]. In case of the SnV^0 and SnV^-, the position of the ZPL shows a smaller dependence on the color center concentration. In contrast, the ZPL shift for SnV centers is larger than the one obtained for the GeV^0 color center [4,5]. We also note that the impact of the charge state is rather non-trivial. The calculated results are discussed within the context of the experimental observation of distributions of ZPL positions for the SnV and GeV centers [3,4]. We highlight some of the pitfalls when comparing calculated and experimental results, and indicate how further experimental-theoretical studies can provide insights into the black box of experimentally doped samples [4,5].

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