Calculation of optical properties of defect centers in diamond

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We present results of calculated optical properties of extended and nanoscale diamond structures with embedded defect centers in different charge states (nitrogen-vacancy (NV), silicon-vacancy (SiV), germanium-vacancy (GeV)). In particular, the chosen defect centers are promising candidates for the realisation of quantum information, quantum processing and high resolution magnetometry technologies. These applications require precise prediction of optical properties of defect centers seperated by less than 10nm where quantum entanglement becomes significant. Using standard density funtional theory (DFT) for diamond nanostructures and a new approximate nonself-consistent method based on atomistic effective potentials (AEP) for extended diamond bulk systems, ground state calculations have been performed. Taking the (effectively) LDA wave functions as a starting point, we model many body effects on the defect transitions using a configuration interaction approach combined with an empirical screening. Furthermore, the screened Coulomb integrals include a treatment with a mask function which take the vacancy screening into account.
Results of optical spectrum calculations of extended diamond systems (bulk) with an embedded isolated negatively charged NV defect (NV^-) to systems containing 2 NV^- placed at different distances to each other are compared. Furthermore, defect free diamond nanostructures passivated with hydrogen atoms are discussed, in particlar, surface states appearing in the bandgap. Placing impurities into these nanostructures lead to additional bandgap states which are characterstic for each defect. Their influence on the many-body optical spectrum is analysed and discussed.