Investigations on optical properties of the nitrogen-vancancy centre

D. Antonov,[1,2] G. Bester,[2] and J. Wrachtrup[1]

[1] *3. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany*
[2] *Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany*

We present theoretical calculations of the optical properties of extended and nanoscale diamond structures with embedded nitrogen-vacancy centres (NV). In particular the negatively charged NV^- center is a promising system for the realisation of devices displaying quantum information, quantum processing and high resolution magnetometry. For these applications a precise prediction of the optical properties of entangled NV^- centers seperated by less than 10nm is required. Utilising a new *ab-initio* method with local density approximation (LDA) accuracy based upon atomistic effective potentials (AEP), spin-polarised calculations of large scale diamond systems have been performed. Additionally, configuration interaction has been used post hoc to obtain excitation spectra. The results of the energy spectra at the many body level confirm group theory predictions. Furthermore, the obtained level scheme for the NV^- is in good agreement with experimentally obtained optical transitions.