Machine learned spin-phonon coupling in Nitrogen-Vacancy centers

Johannes Gugler, Martin Pimon, Matthias Ebert, Paul Worm and Peter Mohn

Center for Computational Material Science, Institute of Applied Physics, TU Wien

Introduction: The negatively charged Nitrogen-Vacancy center (NV^- center) in diamond is a workhorse for applied quantum physics. Its possible application as a Qubit depend on the excellent spin-properties of the system. The system exhibits exceptionally long spin-lattice relaxation times T1 for electron spins[1], which could be explained in the low temperature regime by the calculation of spin-lattice relaxation in first order perturbation theory on a quantum mechanical level using density functional theory (DFT)[2]. Since high temperature applications would be very useful, an understanding of higher order perturbations is needed. However, due to the large phase space to be sampled, the number of necessary calculations outreaches the capabilities of modern computer clusters. Hence, we are trying to use machine learning methods for the treatment of the structures and the behaviour of the electron spin, if the atoms next to the NV^- center are moving.

The defect is also used as a very precise atomic measurement tool: The easy C_{3v} symmetry allows for a precise description of the influence of external magnetic and electric fields and thus to measure these fields with probing the transitions of the defect states. In addition, the spin-properties of the system are temperature dependent, which makes the application of an atomic sized temperature sensor possible[3].

Method: Based on our predictive machine learning approach, we will be able to reduce the number of DFT calculations to extract the necessary information for our neural network by learning spin-phonon coupling. With the learned coupling constants in our hand, we will use second order time dependent perturbation theory and calculate the spin-lattice relaxation time T1 at room temperature. Also, we simulate thermal ensembles to extract the temperature dependence of the spin-properties to give a profound description of the system and pave the way towards an accurate atomic sized temperature sensor.

References

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