Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Simulation of Diamond Based Quantum Token

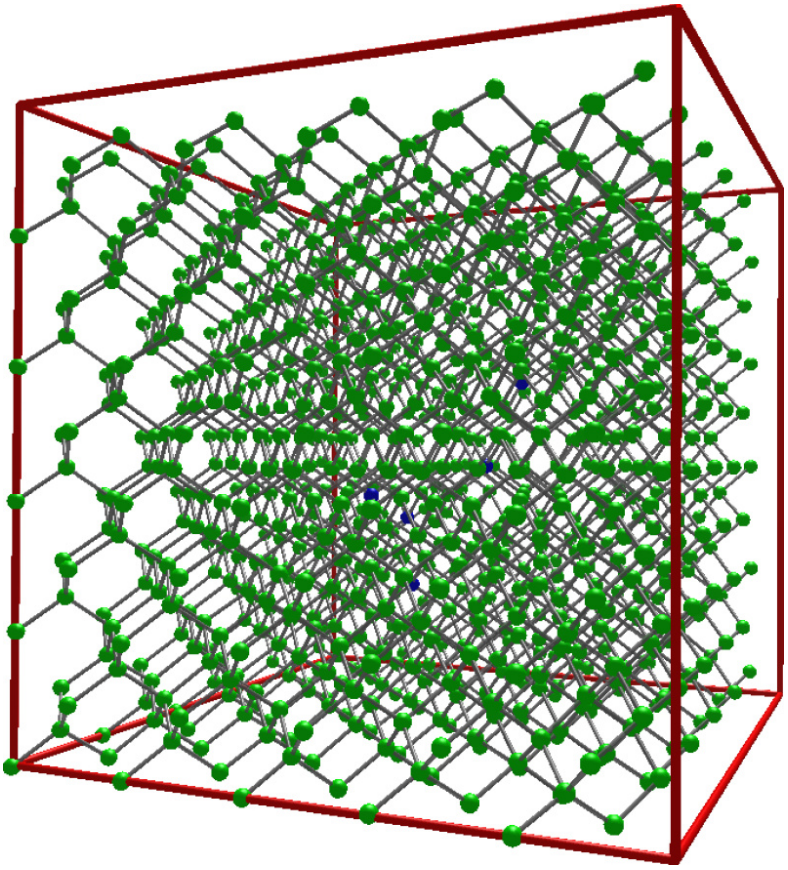


Figure 1: Bulk supercell with 986 carbon (green) 5 nitrogen (blue) and 9 vacancies is shown.

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Clusters
Lichtenberg Cluster Darmstadt

Additional Software
CHIVES

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Introduction

NV centers – a nitrogen atom together with a vacancy – embedded in diamond provide a promising system to generate quantum tokens. Reason for this is that the NV center exhibits electronic states like a single atom and these states are very stable due to the embedding in the diamond lattice. Lasers can be used to manipulate the electronic state of a NV center. Using diamond nano pillars one can maximize the light intensity, which penetrates the diamond and reaches the NV center. The great challenge is the generation of the NV centers in diamond: Nitrogen atoms can be shut into diamond by ion bombardment and vacancies are always present. But after the bombardment the nitrogen atoms are far away from the vacancies. Previous T_e-dependent density functional theory calculations in our group showed that an excitation by a femtosecond laser pulse induces a movement of a nitrogen atom to a vacancy, so that a NV center is formed. This indicates that the hot electrons remove barriers in interatomic bonding, so that the nitrogen atom moves through the lattice to the vacancy. In order, to perform simulations of the NV center formation in diamond nano pillars, one has to consider millions of atoms. This is only possible by using a T_e-dependent interatomic potential and high-performance computer (HPC) facilities.

Methods

In order to construct a reasonable T_e-dependent interatomic potential, one needs a large data set of T_e-dependent density functional theory calculations. We derived a molecular dynamics code based on Mermin's electronic-temperature-dependent density functional theory. Our Code for Highly-excIted Valence Electron Systems (CHIVES) uses local basis sets for treating the valence electron system and norm-conservation pseudopotentials for the core electrons. CHIVES can be used efficiently on a HPC system due to usage of OpenMP and MPI parallelization in the code. We could show for a highly non-symmetric atomic configuration that CHIVES used to be about two hundred times faster than state-of-the-art plane-wave codes.

Results

Using our code CHIVES, we generated within this project a large data set of T_e-dependent DFT calculations in order to get a rich sample of the potential energy surface. In detail, we performed MD simulations of a diamond bulk supercell and of a thin diamond film containing one NV center. In addition, we took the thermalized diamond bulk structure with 1000 carbon atoms and placed randomly nitrogen atoms and vacancies. One of these configurations is shown in Figure 1. Using these atomic configurations, we set randomly velocities to the atoms and used these atomic velocities and coordinates as initialization for molecular dynamics (MD) simulations at various electronic temperatures. After some timesteps of these MD simulations, we took the actual atomic coordinates and set new randomly generated velocities as initialization for additional MD

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simulations. We also generated a thin diamond film with 1280 carbon atoms and placed randomly nitrogen atoms and vacancies and calculated the corresponding atomic forces and cohesive energies.

Discussion

Using the generated ab-initio dataset, we will be able to construct the T_e-dependent interatomic potential describing diamond with NV centers included.

Publications

Bauerhenne, B.; Xibraku, M.; Garcia, M. E.: ”TTM-MD simulations compared with experiments”, Diqtok Kickoff meeting, 10.06.2022, Kassel.

Reference

Bauerhenne, B.; Xibraku, M.; Plettenberg, P.; Garcia, M.E.: ”Machine Learning based Interatomic Potentials to Describe Laser-Excited Materials”, Ultrafast Surface Dynamics, 27.05.2022, Benasque Spanien.

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