### The diamond NV-center

- Color center containing atomic nitrogen and a vacancy situated on neighboring vacancy positions.
- Formed by irradiation (creating vacancies), followed by annealing (make vacancies move to nitrogens).
- Can be in a neutral or negative state. The negative state is the most well researched and promising.
- Exhibits a zero-phonon line at 1.945 eV under optical excitation.
- The process of optical excitation and decay results in a preferential occupation of the $S_z = 0$ ground state level.
- Have long spin lattice lifetime.
- The two previous properties makes the NV-center a promising candidate for quantum information applications.

### Distance to donor nitrogen in a supercell

- How the electronic levels shift when varying the distance to the electron donor nitrogen.
- At what distance the NV-center is "destroyed" (shifting more than 20 percent).
- Placing donor N on the C$_3$ symmetry axis or perpendicular (on the side) to C$_3$.

### Different types of surfaces and terminations

- (001), (110) and (111) oriented surfaces investigated.
- Terminations include H, F, OH and clean.
- Reconstructed surfaces.
- Putting a molecule on surface.

### HSE06 vs PBE

- DFT underestimates the bandgap.
- Using HSE06 to widen the bandgap.
- Experimental bandgap of bulk diamond is 5.4 eV.
- PBE gives 4.171 eV.
- HSE06 gives 5.268 eV.

### Conclusions and future work

- N-N distance influence transition energies.
- Need to use HSE06 instead of PBE.
- Study the NV-center interaction with other diamond defects breaks N.
- Study how the NV-center interact with different functionalizations of the surface.

### Acknowledgements

- Swedish Research Council.
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- HPCIN.
- PDC.
- JVC.

### Surfaces, slab calculations

#### Table 1: PBE Energies (eV), large diamond slabs with NV defect

<table>
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<tr>
<th>Surface</th>
<th>Termination</th>
<th>N-N dist (Å)</th>
<th>Atom</th>
<th>Energy gap (eV)</th>
<th>Workfunction (up)</th>
<th>Workfunction (down)</th>
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</thead>
<tbody>
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<td>100 atom</td>
<td>304 atoms, 20 layers</td>
<td>5.0486</td>
<td>1.894</td>
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### Graphs and Figures

- Figure 1: Energy levels belonging to the NV-center.
- Figure 2: Transition energy between v and e levels for NV-N configuration in 512 atom supercell.
- Figure 3: Transition energy between v and e levels for NV-center in bulk diamond at different N-N distances.
- Figure 4: The groundstate A$_g$, the excited state E, and the ZPL corresponding to the v-e transition.
- Figure 5: The groundstate A$_g$, the excited state E, and the ZPL corresponding to the v-e transition.
- Figure 6: Transition energy between v and e levels for NV-center in bulk diamond at different N-N distances.
- Figure 7: The diamond NV-center.
- Figure 8: (100), (110), and (111) surfaces.
- Figure 9: Workfunction for a small 16-carbon atom F-terminated (110) surface.