

Ab initio studies of vacancy-impurity complexes in cubic and hexagonal diamond

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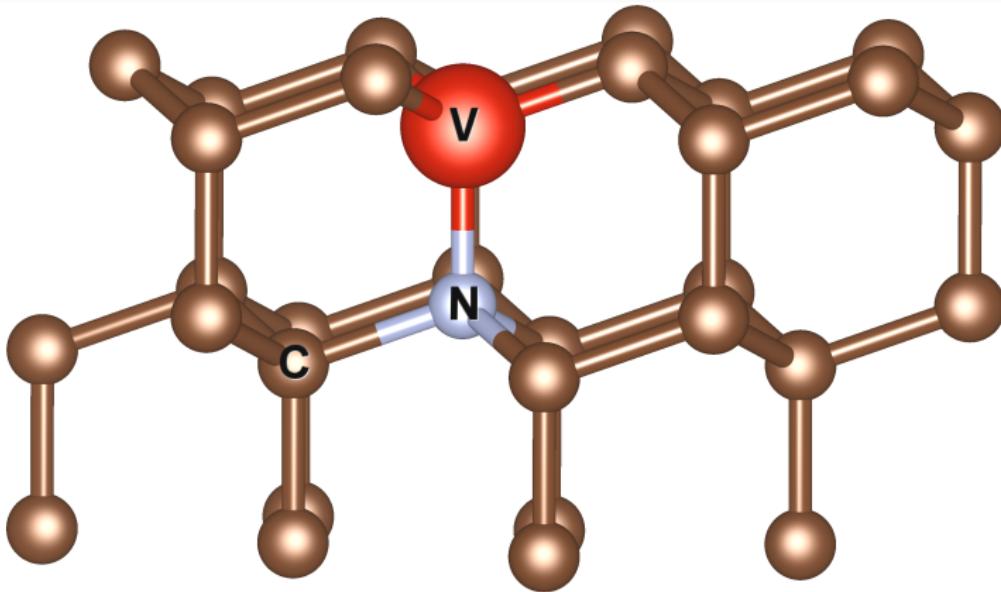
Aim and scope of the work

Aims

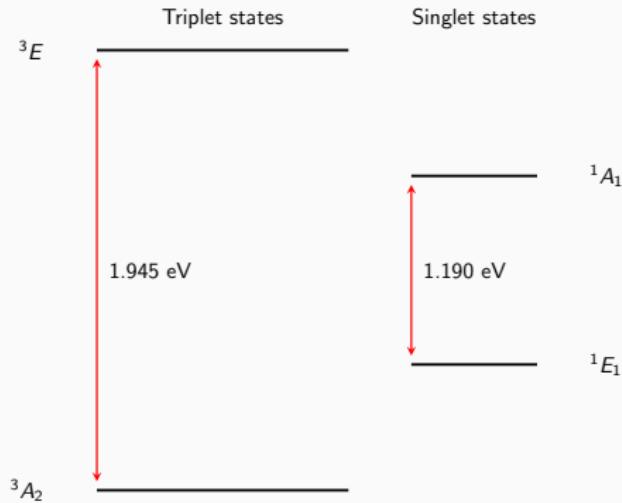
- Exploration of defect centres using state-of-the-art ab-initio theories.
- Reproduce and obtain classical results for nitrogen vacancy impurity complexes in diamond.

Introduction

Nitrogen Vacancy Centre in diamond

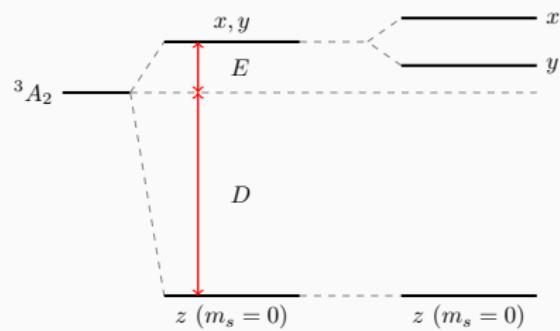


Main level overview: NV⁻

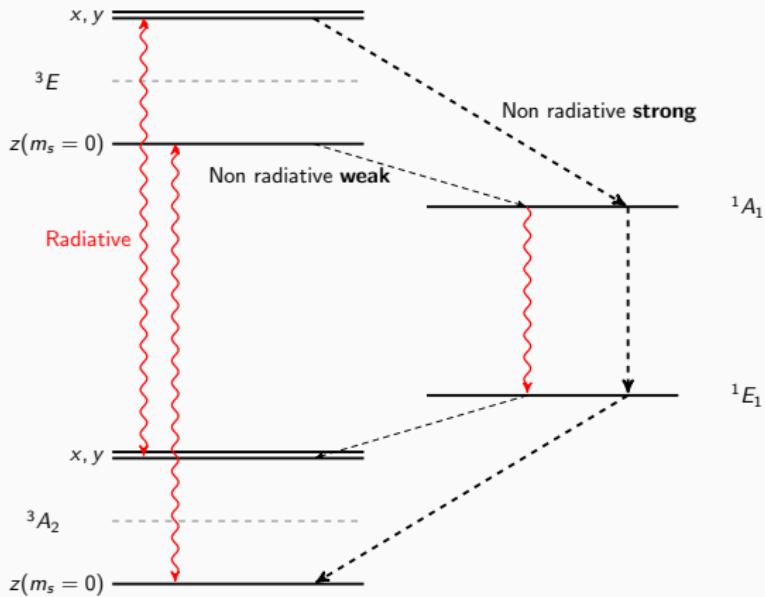


Transitions

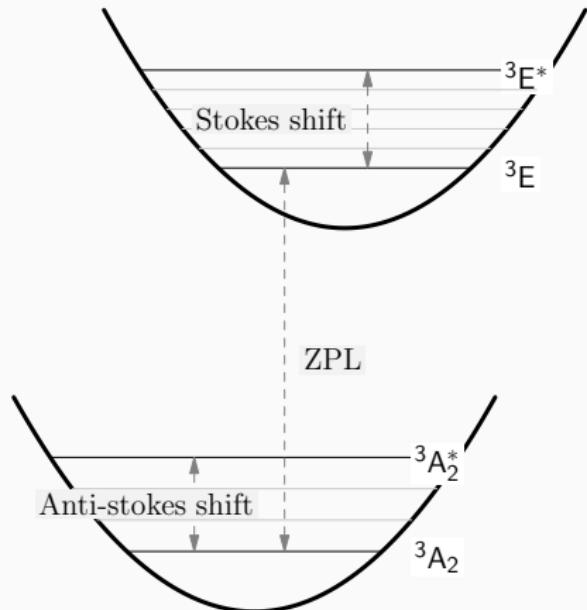
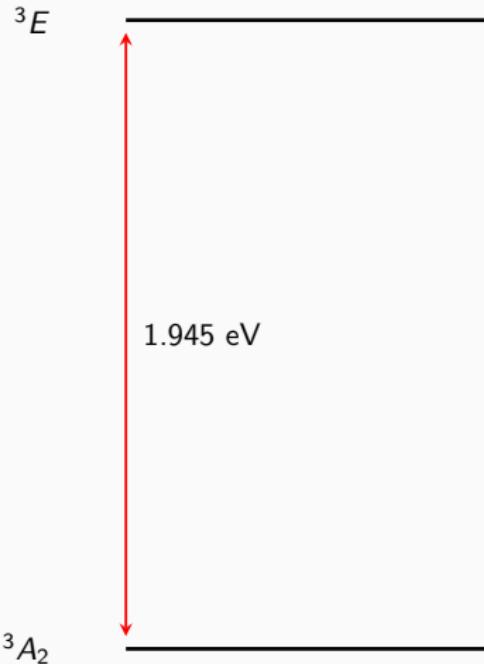
$\hat{S}^t D \hat{S}$ Zeeman/strain



Transitions overview: NV⁻



Zero phonon line (ZPL)



Density functional theory (DFT)

" Ψ contains too much information"

- Popular saying

- The exact electronic ground state of a system is only dependent on the electronic density ρ .
- In principle, DFT delivers the **exact ground state**.
- All quantities written in terms of ρ (functional formalism).
- E.g.:

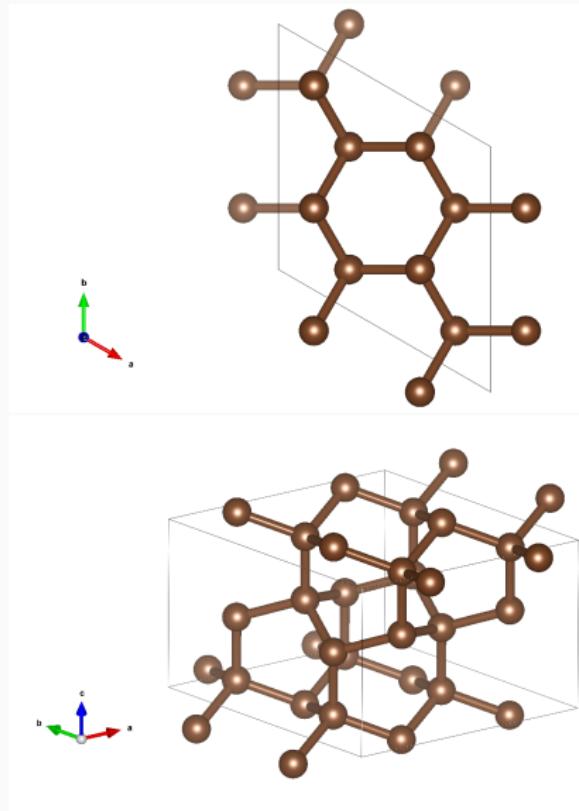
$$E[\rho] = T_s[\rho] + \int V(\mathbf{r})\rho(\mathbf{r}) \, d\mathbf{r} + \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d\mathbf{r} d\mathbf{r}' + E_{\text{xc}}^{\text{exact}}[\rho]$$

The exchange correlation potential $E_{\text{xc}}^{\text{exact}}[\rho]$ determines the DFT flavor.



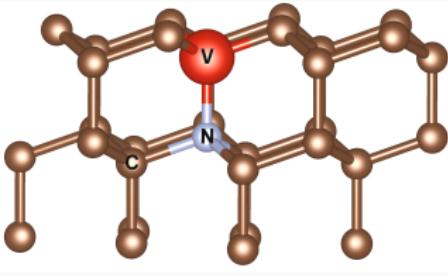
Hexagonal diamond and defects

Hexagonal diamond

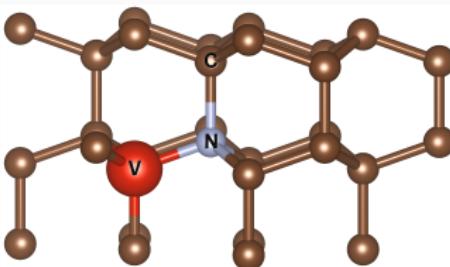


Defected hexagonal diamond

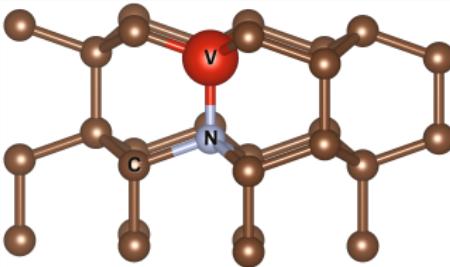
Cubic diamond



Hexagonal x-type



Hexagonal z-type

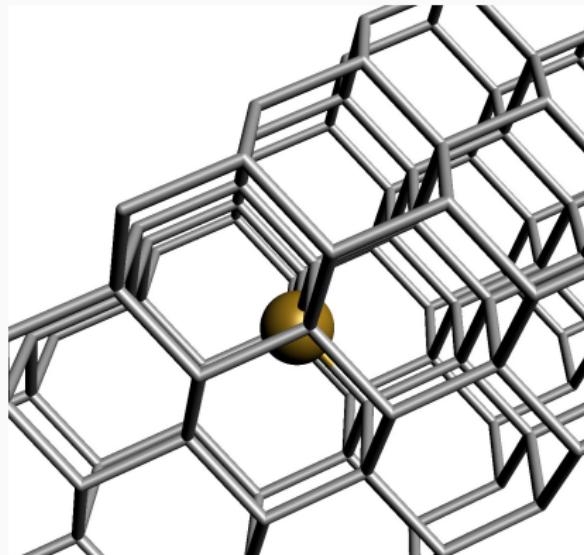
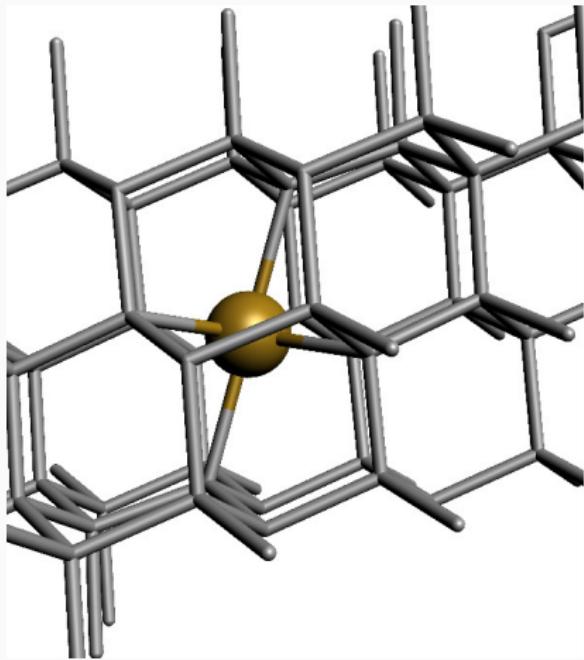


Expanding the defect

| 18 VIII A | | | | | | | | | | | |
|-----------|-------------|-------------|-------------|-------------|------------|------------|--------|-------------|-------------|------------|------------------|
| 13 IIIA | | 14 IVA | | 15 VA | | 16 VIA | | 17 VIIA | | He | |
| 5 | 10.811 | 6 | 12.011 | 7 | 14.007 | 8 | 15.999 | 9 | 18.998 | 10 | 4.0025 Helium |
| B | Carbon | C | Nitrogen | N | Oxygen | O | | F | Flourine | Ne | Neon |
| Boron | | Carbon | | Nitrogen | | Oxygen | | Flourine | | Neon | |
| Al | Silicon | Si | Phosphorus | P | Sulphur | S | | Cl | Chlorine | Ar | Argon |
| Aluminium | | Silicon | | Phosphorus | | Sulphur | | Chlorine | | Argon | |
| Ga | Germanium | Ge | Arsenic | As | Selenium | Se | | Br | Bromine | Kr | Krypton |
| Gallium | | Germanium | | Arsenic | | Selenium | | Bromine | | Krypton | |
| In | Tin | Sn | Antimony | Sb | Tellurium | Te | | I | Iodine | Xe | Xenon |
| Indium | | Tin | | Antimony | | Tellurium | | Iodine | | Xenon | |
| Tl | Lead | Pb | Bismuth | Bi | Polonium | Po | | At | Astatine | Rn | Radon |
| Thallium | | Lead | | Bismuth | | Polonium | | Astatine | | Radon | |
| Uut | Ununquadium | Uug | Ununpentium | Uup | Ununhexium | Uuh | | Uus | Ununseptium | Uuo | Ununoctium |
| Ununtrium | | Ununquadium | | Ununpentium | | Ununhexium | | Ununseptium | | Ununoctium | |

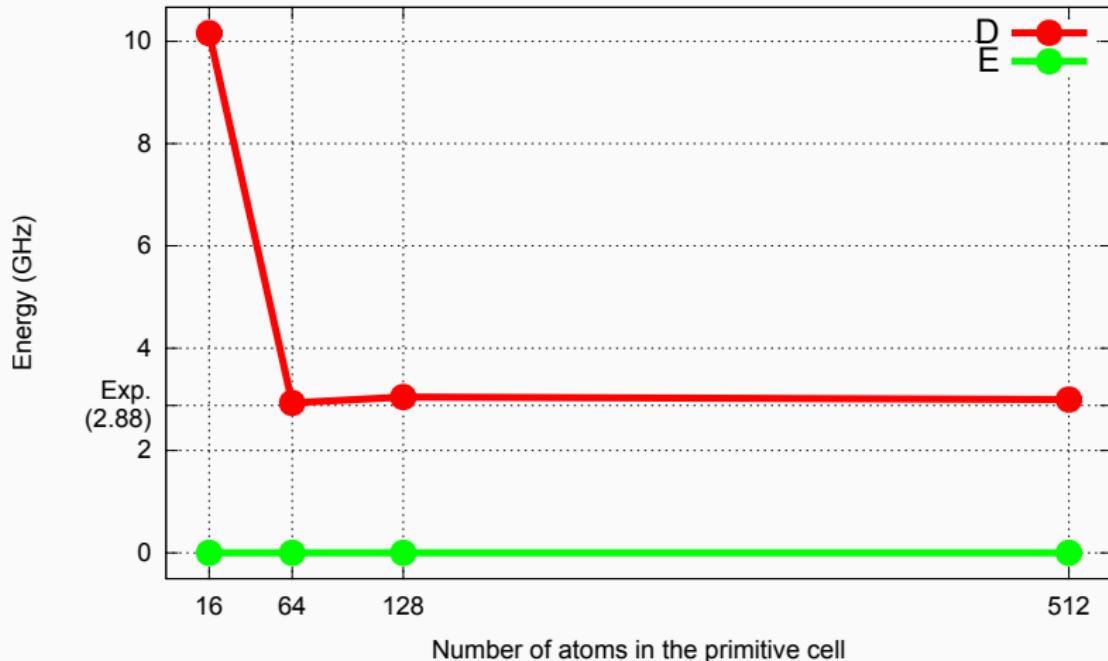


Split vacancies: SiV⁻



Results

ZFS in NV⁻



Recovering experimental results

Summary

Where we are, and where to go next...

- Structural properties
- ZPL calculation.
- ZFS tensor calculation.
- **Beyond the Ground state:**
Using DMRG for excited state calculations

