

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

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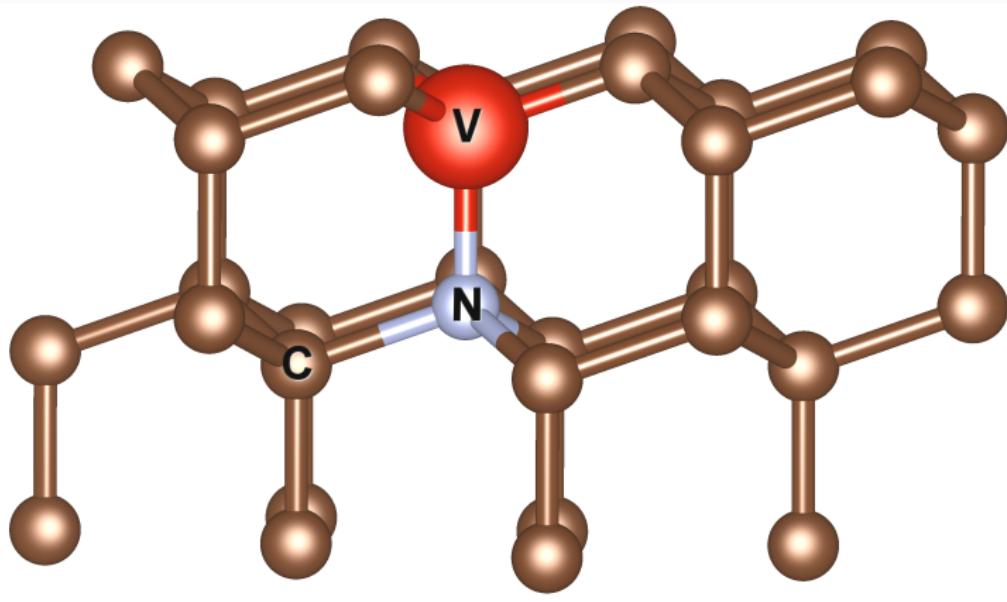
Aim and scope of the work

Aims

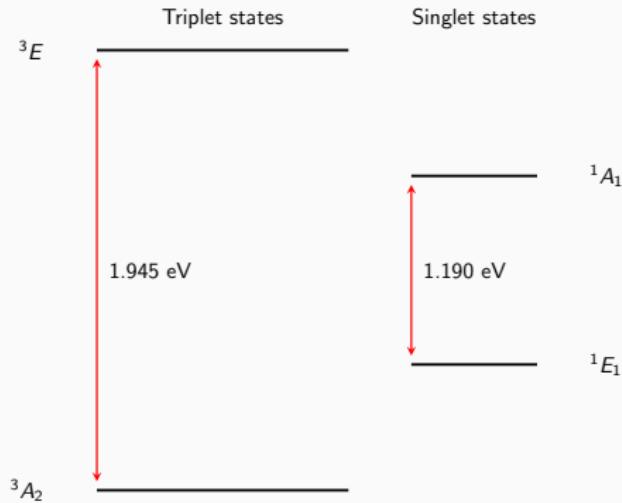
- Exploration of defect centres using state-of-the-art ab-initio theories.
- Reproduce and obtain classical results for nitrogen vacancy impurity complexes in diamond.

Introduction

Nitrogen Vacancy Centre in diamond

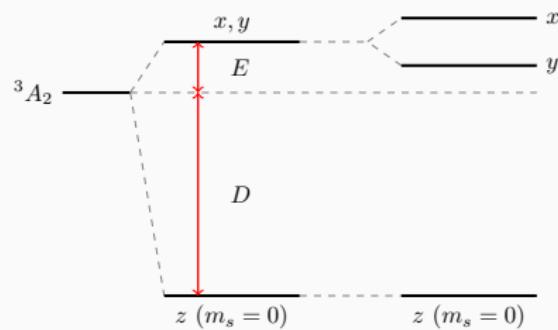


Main level overview: NV⁻

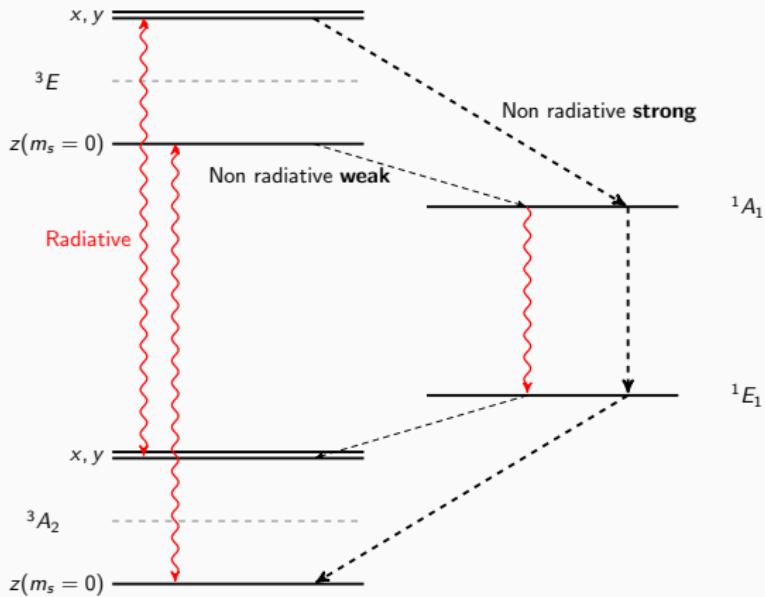


Transitions

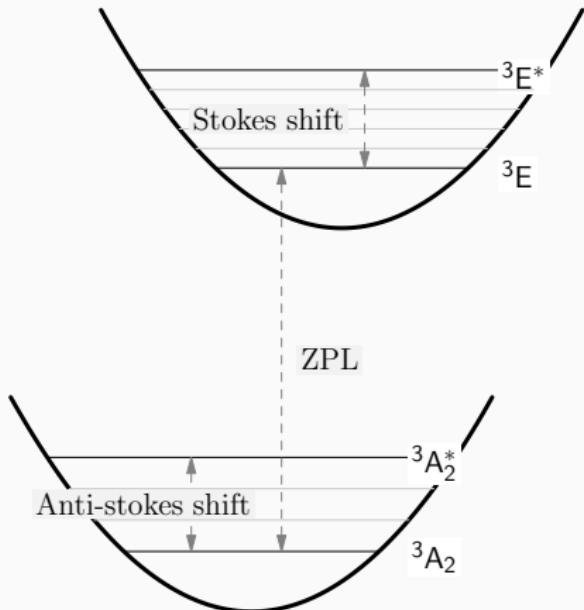
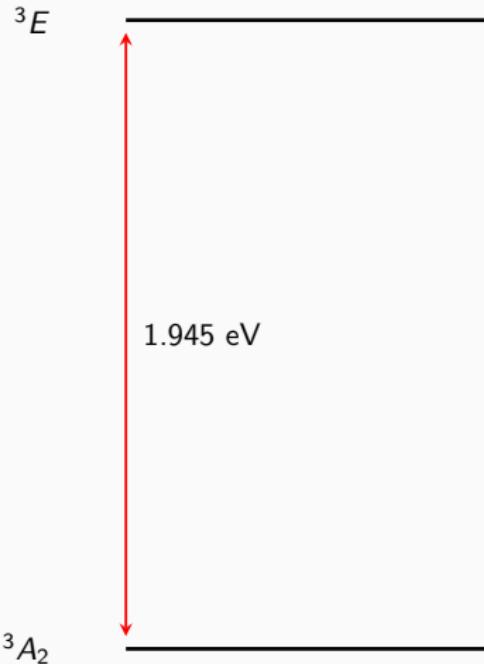
$\hat{S}^t D \hat{S}$ Zeeman/strain



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.:

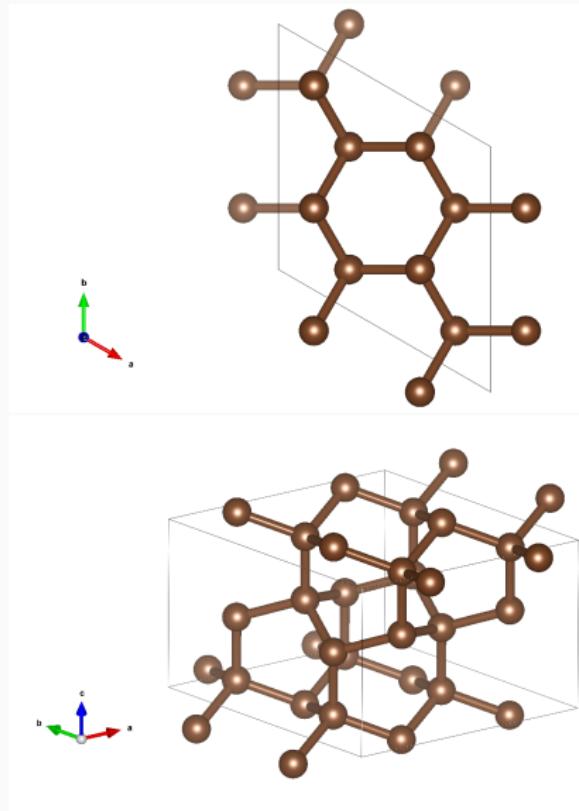
$$E[\rho] = T_s[\rho] + \int V(\mathbf{r})\rho(\mathbf{r}) \, d\mathbf{r} + \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d\mathbf{r} d\mathbf{r}' + E_{\text{xc}}^{\text{exact}}[\rho]$$

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



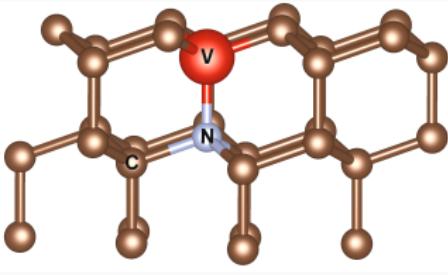
Hexagonal diamond and defects

Hexagonal diamond

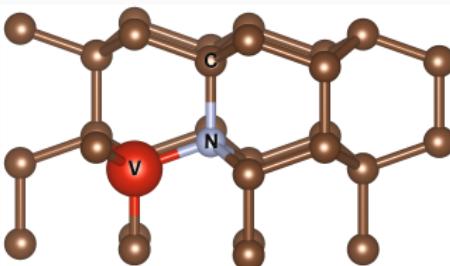


Defected hexagonal diamond

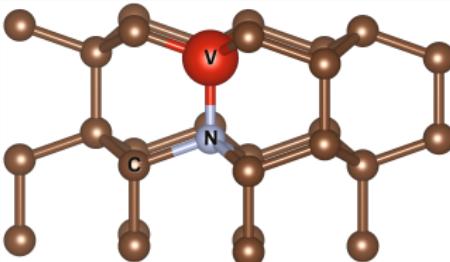
Cubic diamond



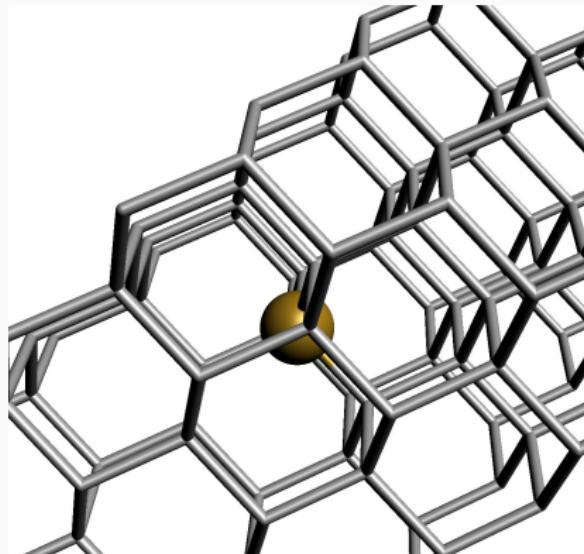
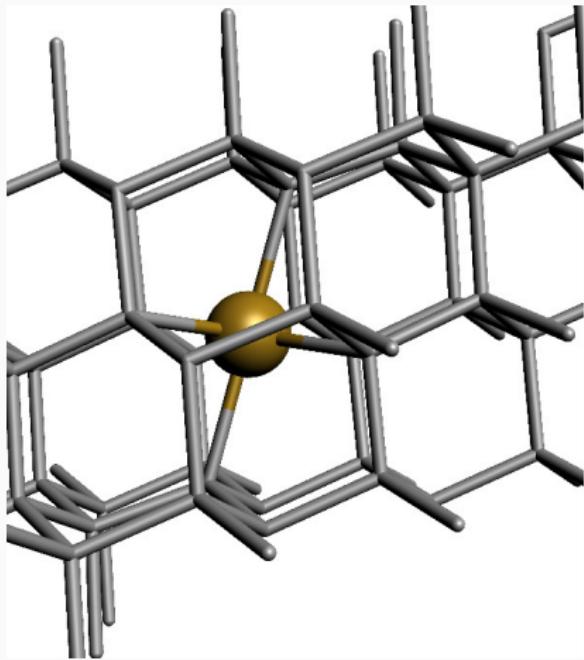
Hexagonal x-type



Hexagonal z-type

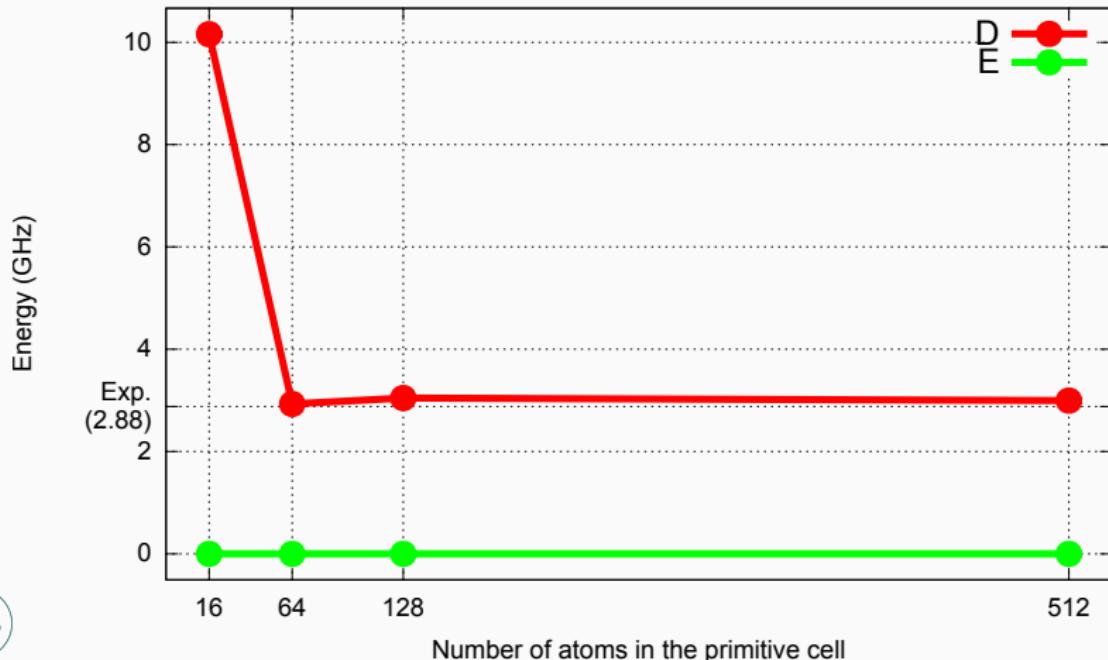


Split vacancies: SiV⁻

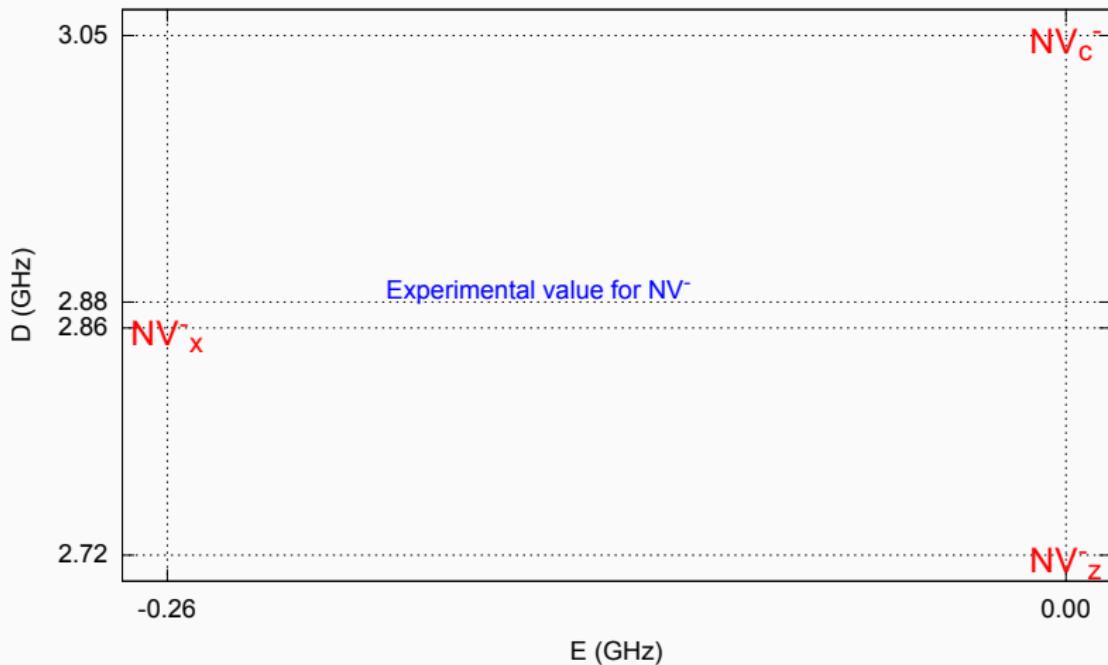


Results

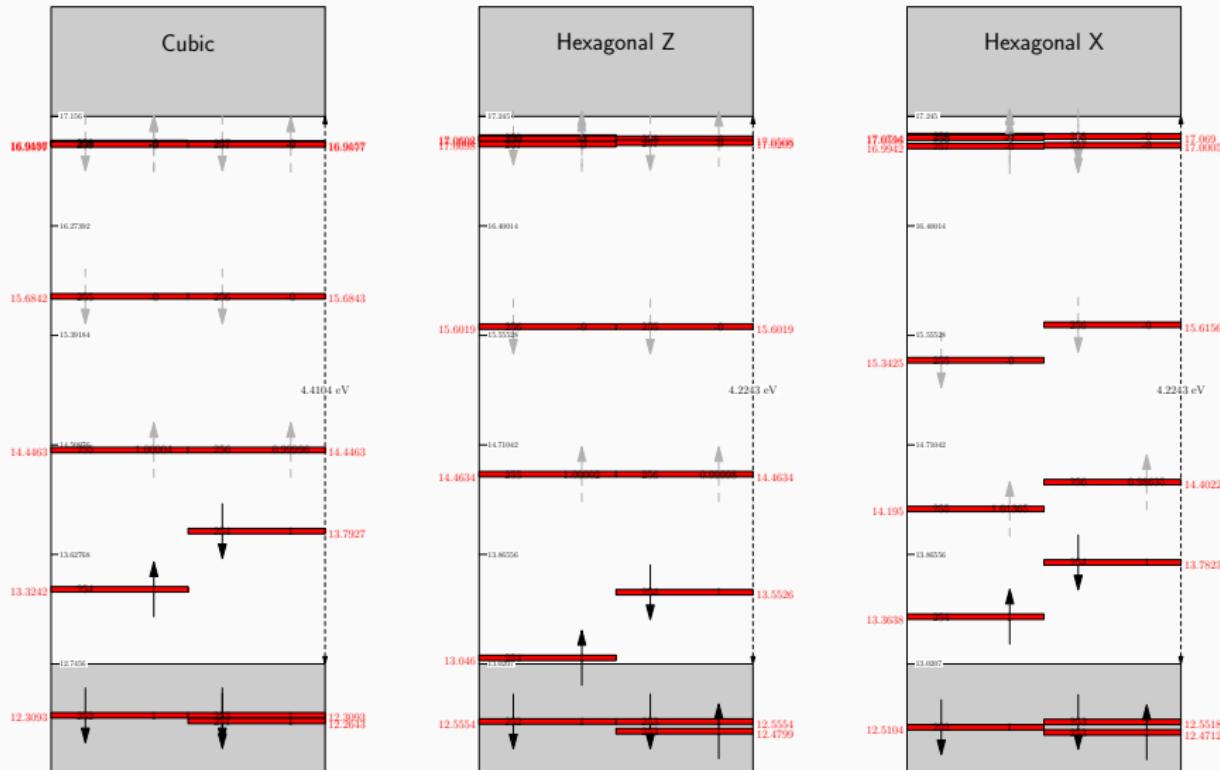
- Cubic diamond, convergence and comparison with the experimental result.



NV*: ZFS cubic (NV_c^*), Hexagonal x, z ($\text{NV}_{x,z}^*$)



NV⁻: Ground state



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	



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

