

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

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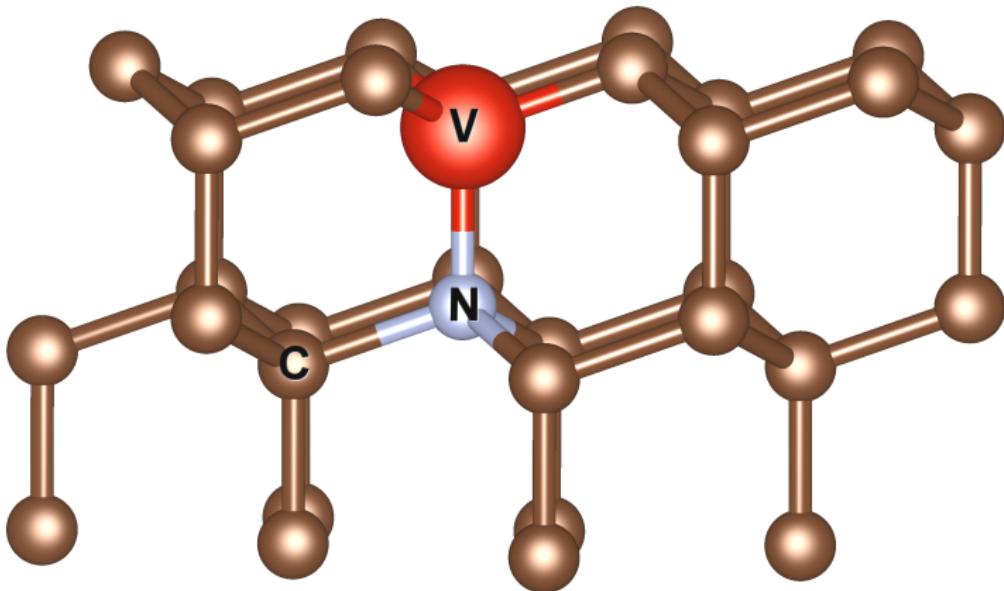
Aim and scope of the work

Aims

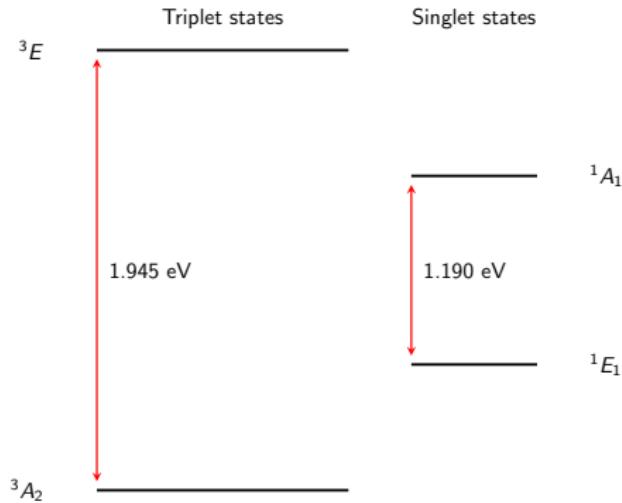
- Exploration of defect centres using state-of-the-art ab-initio theories.
- Reproduce and obtain classical results for nitrogen vacancy impurity complexes in diamond.

Introduction

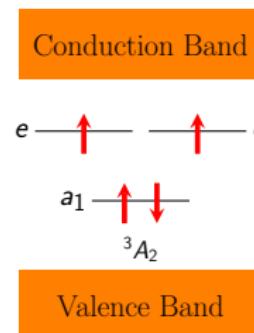
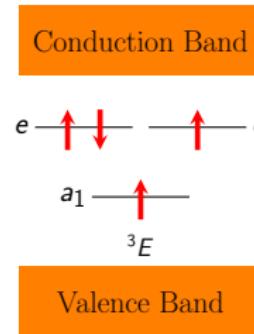
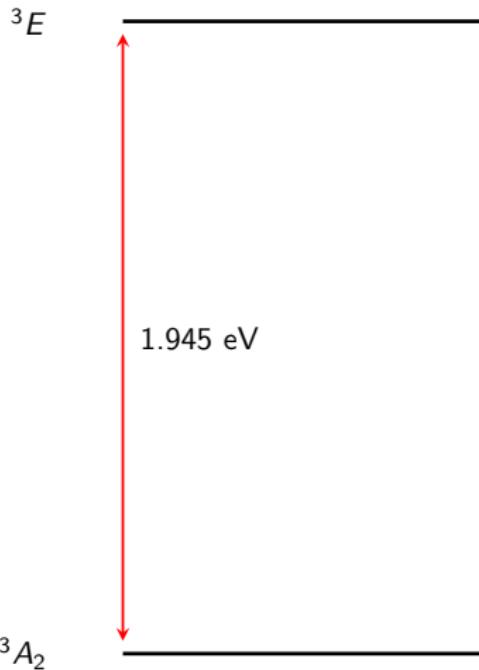
Nitrogen Vacancy Centre in diamond



Main level overview: NV⁻

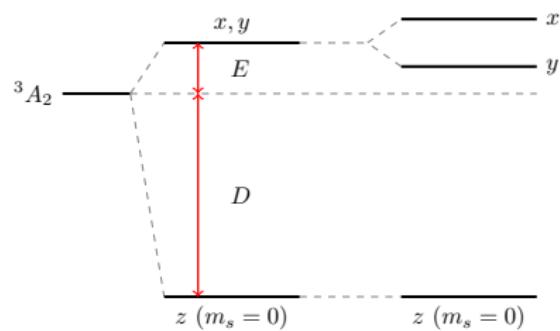


Triplets overview: NV⁻

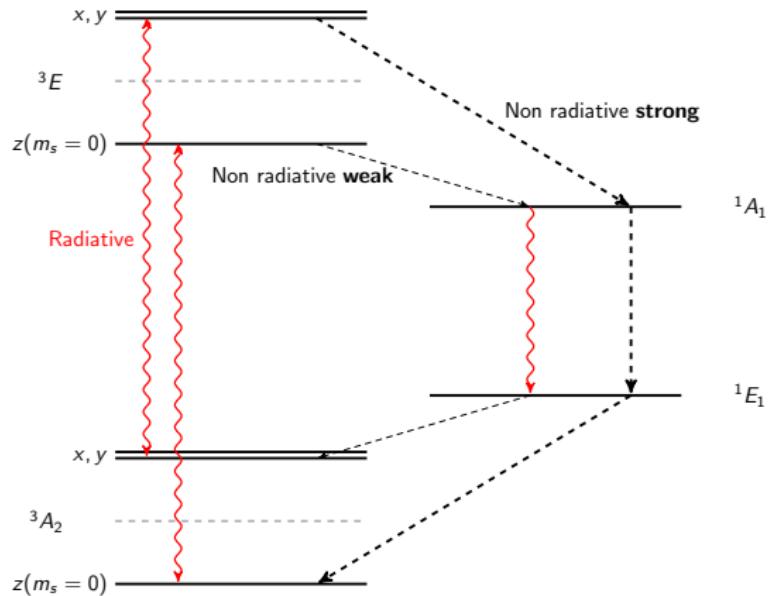


Transitions

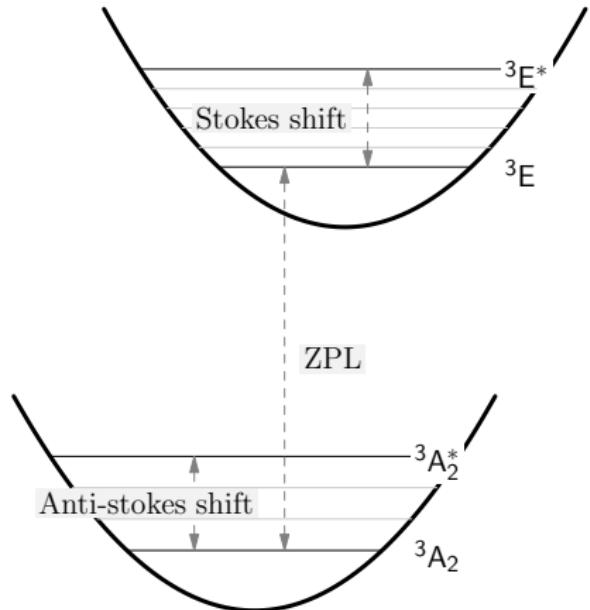
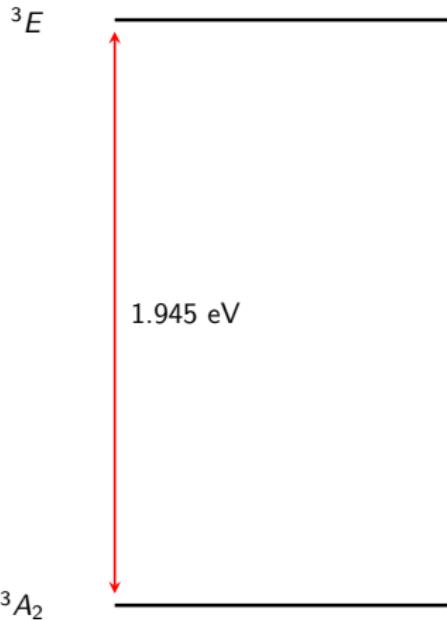
$\hat{S}^t D \hat{S}$ Zeeman/strain



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.:

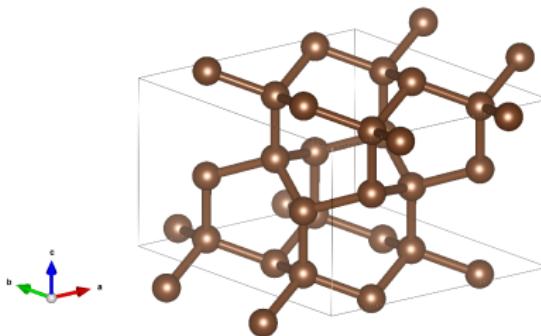
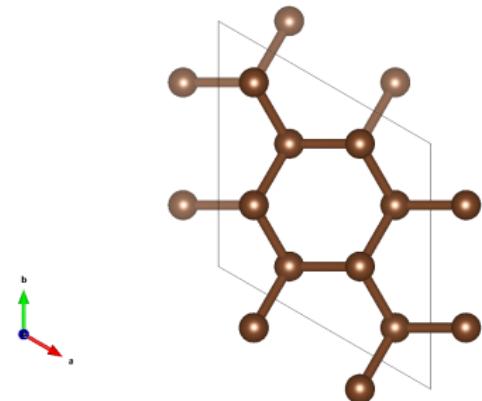
$$E[\rho] = T_s[\rho] + \int V(\mathbf{r})\rho(\mathbf{r}) \, d\mathbf{r} + \frac{1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d\mathbf{r} d\mathbf{r}' + E_{\text{xc}}^{\text{exact}}[\rho]$$

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



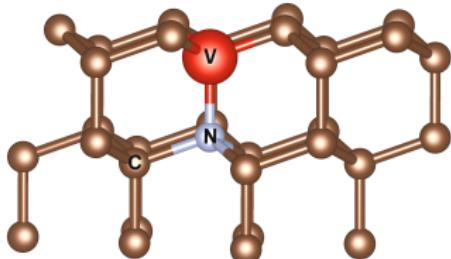
Hexagonal diamond and defects

Hexagonal diamond

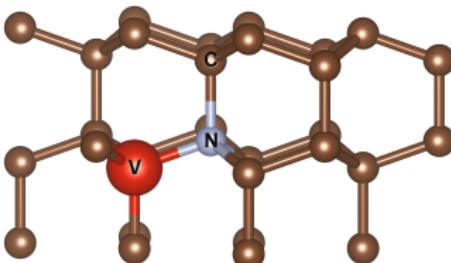


Defected hexagonal diamond

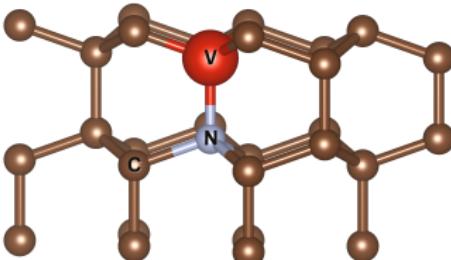
Cubic diamond



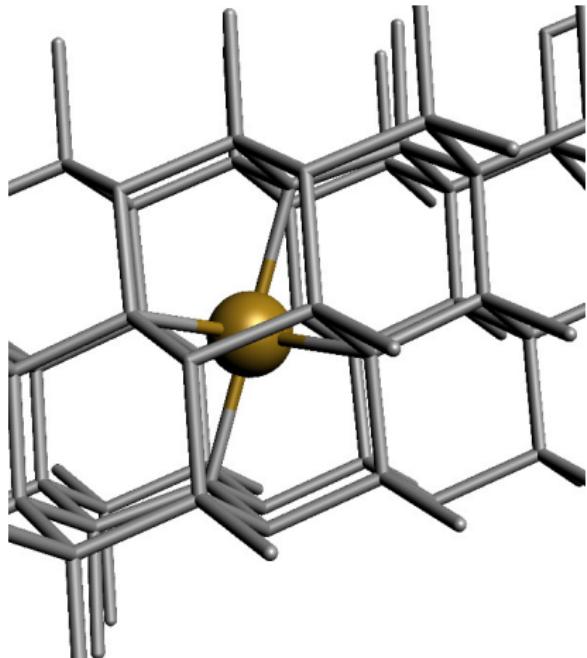
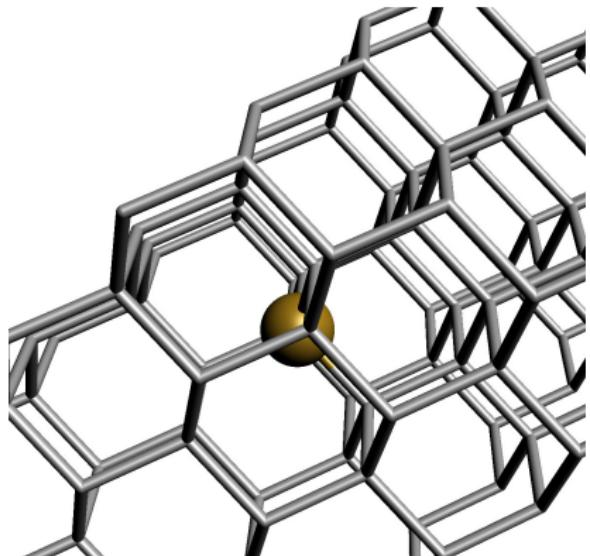
Hexagonal *x*-type



Hexagonal *z*-type

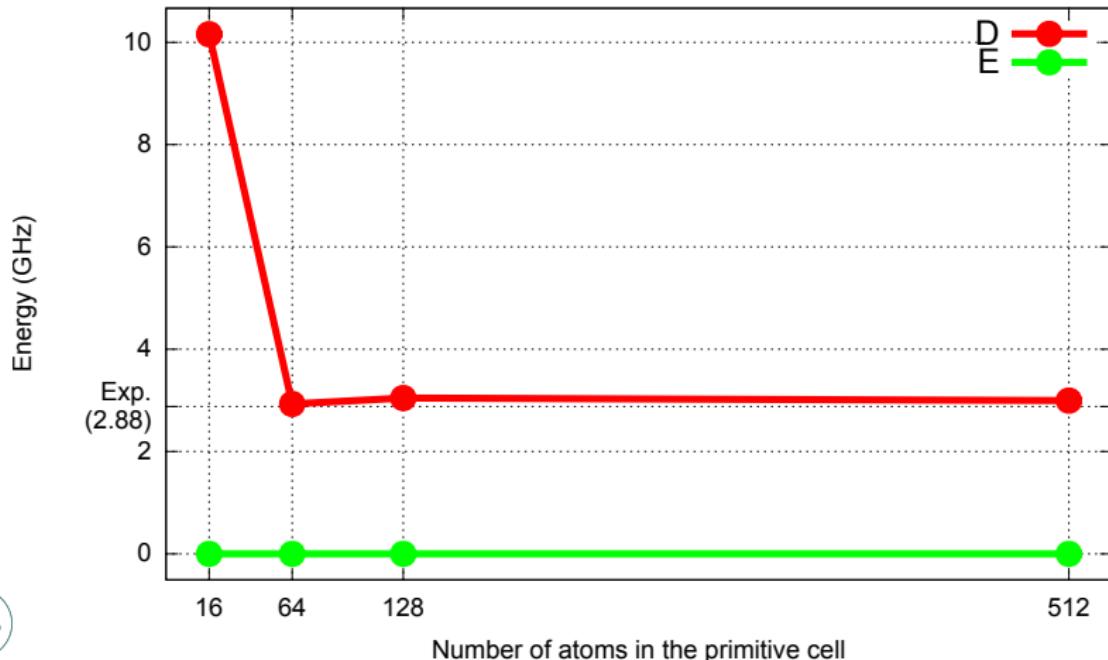


Split vacancies: SiV⁻

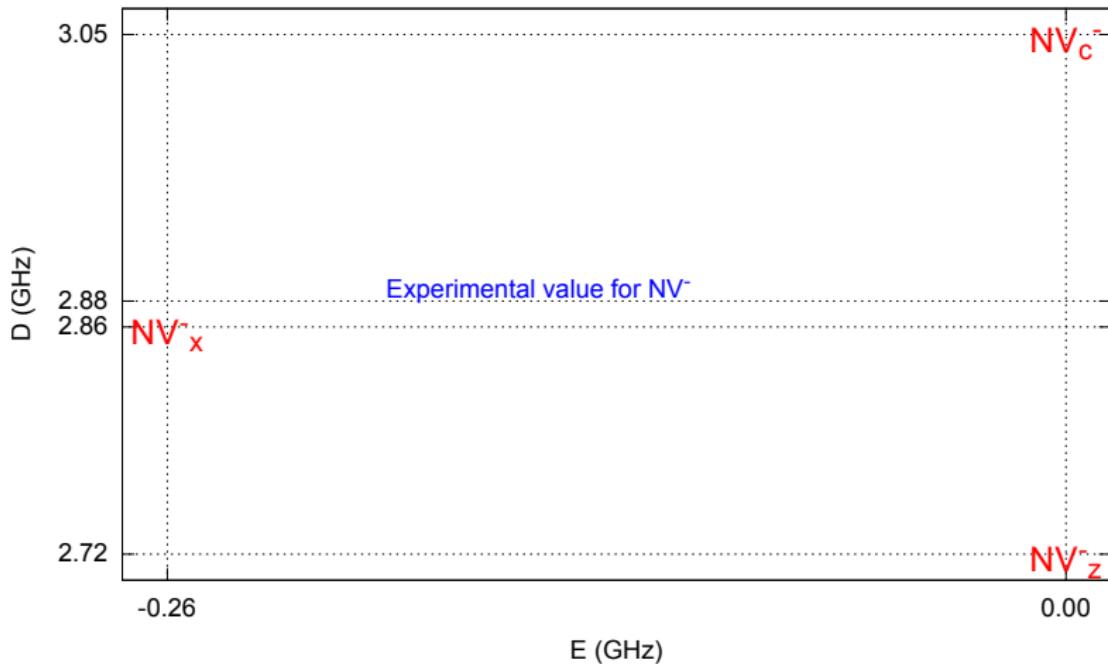


Results

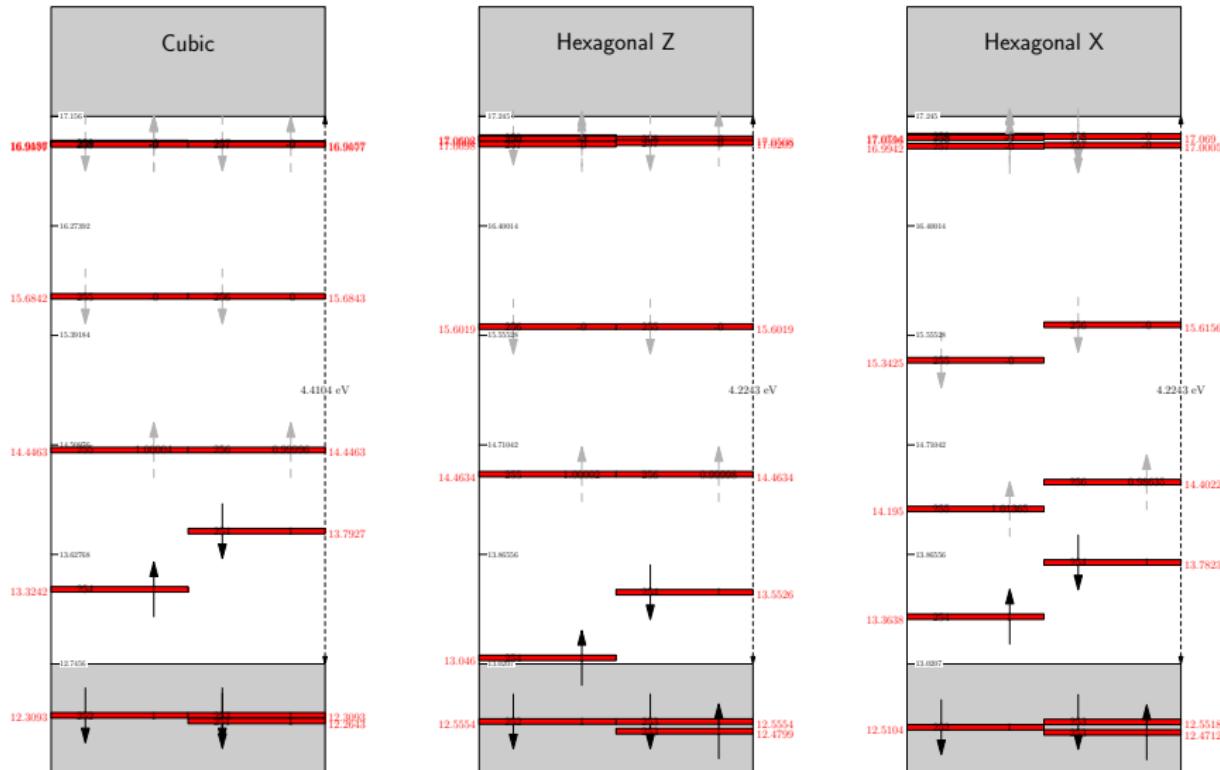
- Cubic diamond, convergence and comparison with the experimental result.



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	
5 B Boron	10.811	6 C Carbon	12.011	7 N Nitrogen	14.007	8 O Oxygen	15.999	9 F Flourine	18.998 10 Ne Neon
13 Al Aluminum	26.982	14 Si Silicon	28.086	15 P Phosphorus	30.974	16 S Sulphur	32.065	17 Cl Chlorine	35.453 18 Ar Argon
31 Ga Gallium	69.723	32 Ge Germanium	72.64	33 As Arsenic	74.922	34 Se Selenium	78.96	35 Br Bromine	79.904 36 Kr Krypton
49 In Indium	114.82	50 Sn Tin	118.71	51 Sb Antimony	121.76	52 Te Tellurium	127.6	53 I Iodine	126.9 54 Xe Xenon
81 Tl Thallium	204.38	82 Pb Lead	207.2	83 Bi Bismuth	208.98	84 Po Polonium	209	85 At Astatine	210 86 Rn Radon
113 Uut Ununtrium	284	114 Uug Ununquadium	289	115 Uup Ununpentium	288	116 Uuh Ununhexium	293	117 Uus Ununseptium	292 118 Uuo 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



Thank you!

