

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

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Aim and scope of the work

Aims

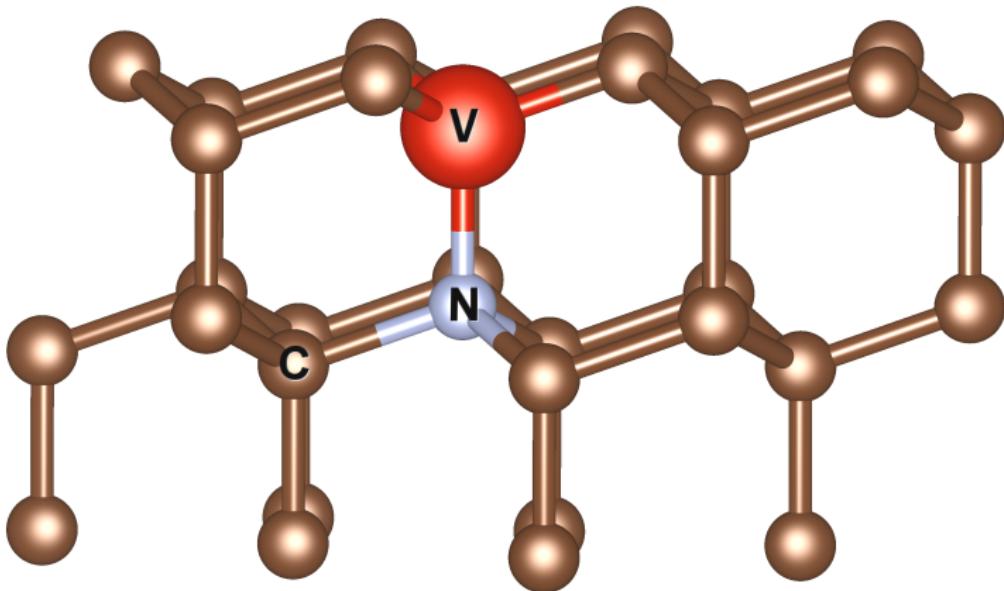
- Exploration of defect centres using state-of-the-art ab-initio theories.

Aims

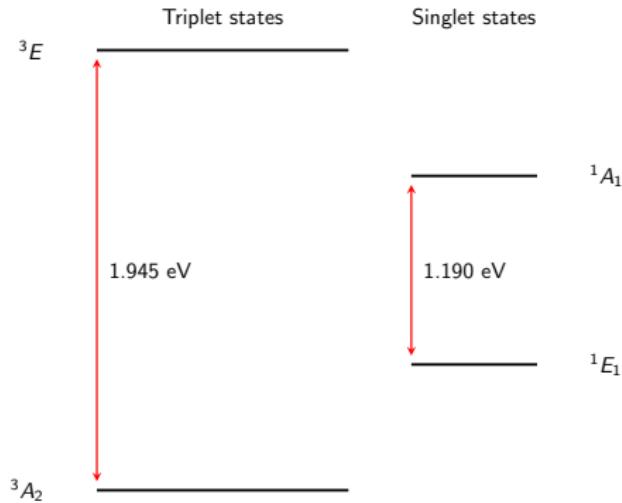
- Exploration of defect centres using state-of-the-art ab-initio theories.
- Reproduce and obtain classical results for nitrogen vacancy impurity complexes in diamond.

Introduction

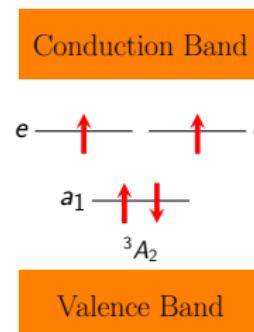
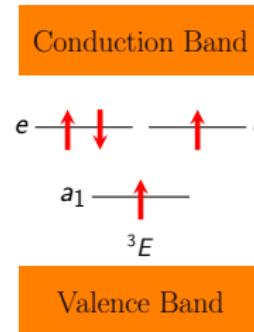
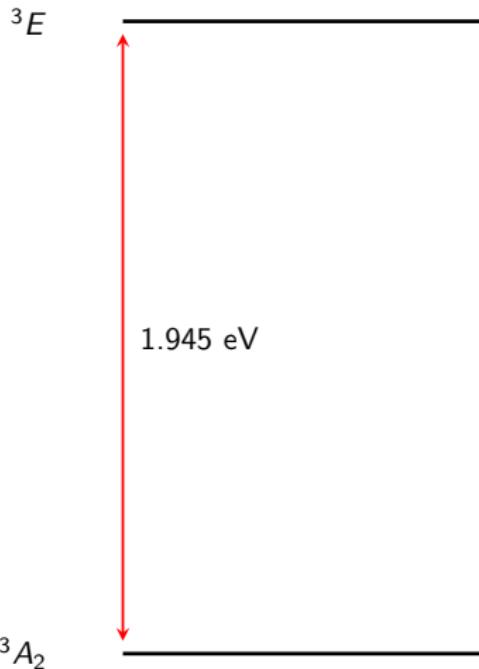
Nitrogen Vacancy Centre in diamond



Main level overview: NV⁻



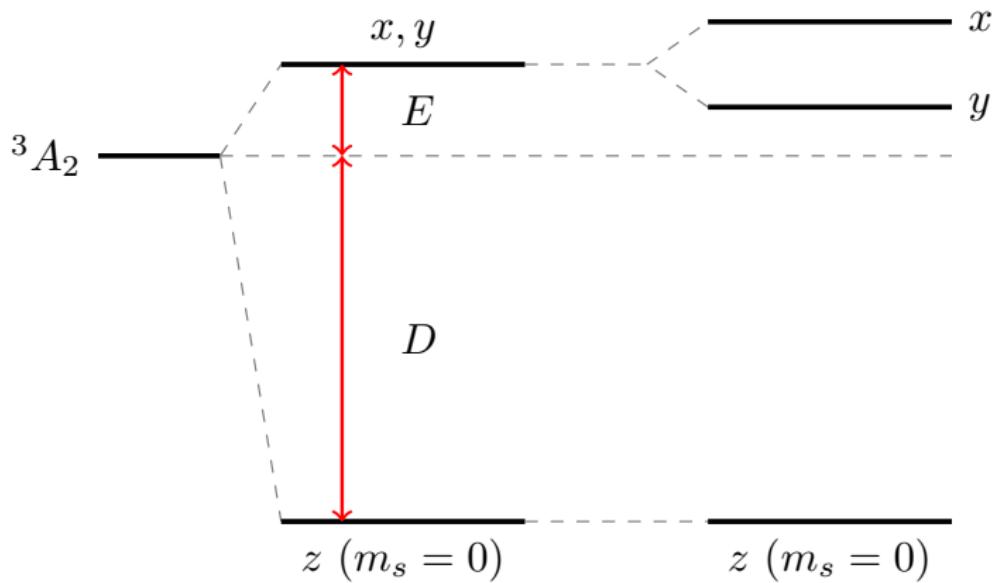
Triplets overview: NV⁻



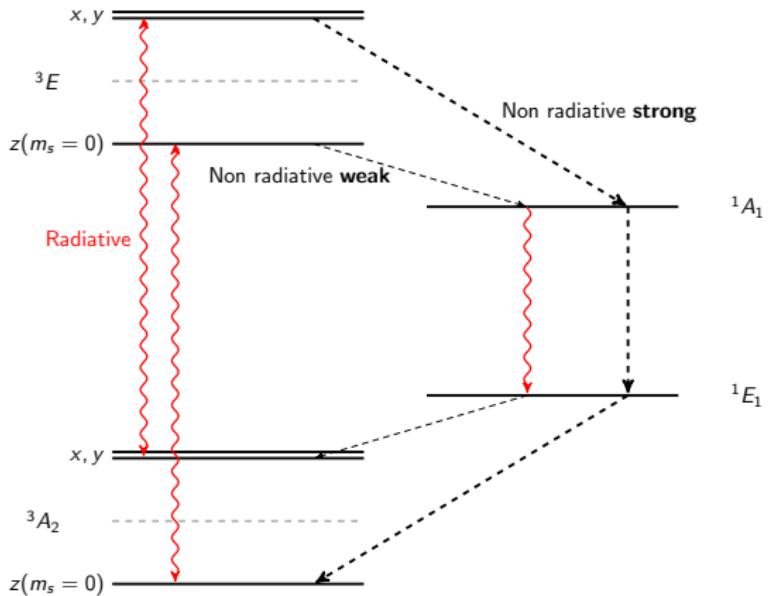
Transitions

$\hat{\mathbf{S}}^t \mathbf{D} \hat{\mathbf{S}}$

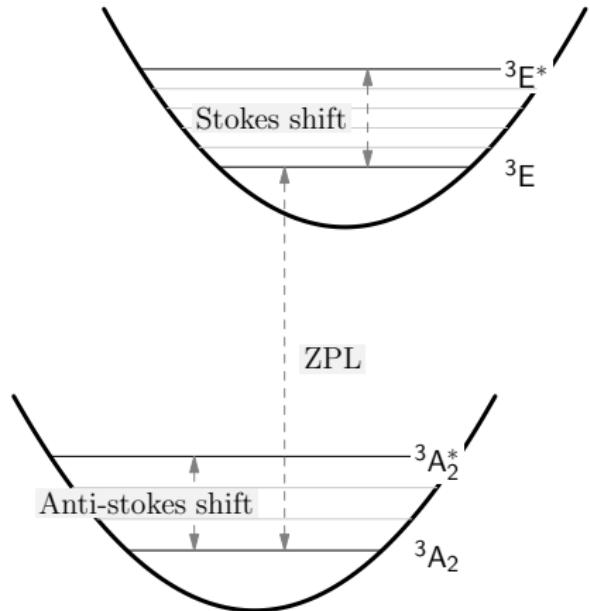
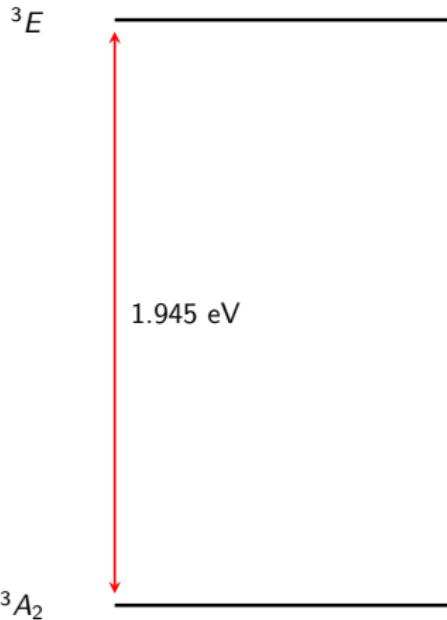
Zeeman/strain



Transitions overview: NV⁻



Zero phonon line (ZPL)



Density functional theory (DFT)

" Ψ contains too much information"

- Popular saying

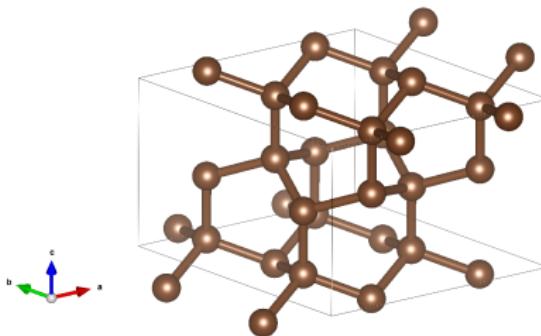
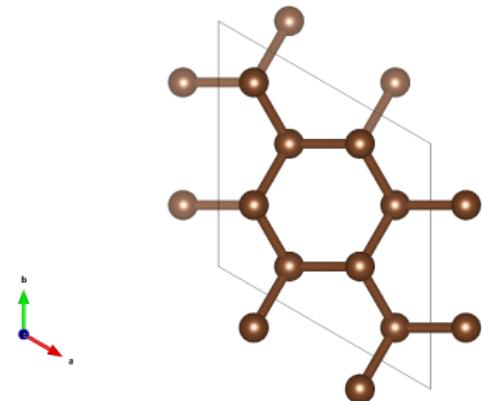
- The exact electronic ground state of a system is only dependent on the electronic density ρ .
- In principle, DFT delivers the **exact ground state**.
- All quantities written in terms of ρ (functional formalism).
- E.g.:

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

The exchange correlation potential $E_{\text{xc}}^{\text{exact}}[\rho]$ determines the DFT flavor. In many calculations we use the so-called **PBE** (*Perdew-Burke-Ernzerhof*) functional.

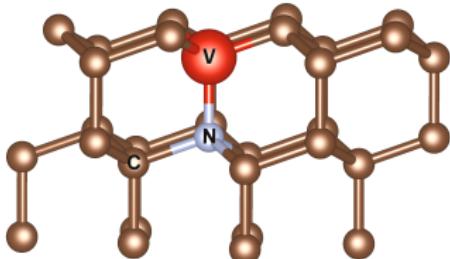
Hexagonal diamond and defects

Hexagonal diamond

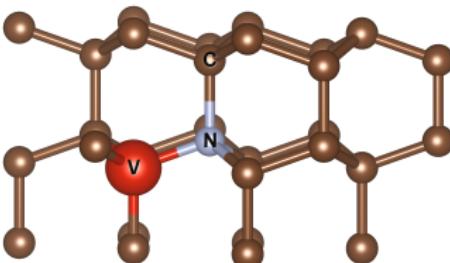


Defected hexagonal diamond

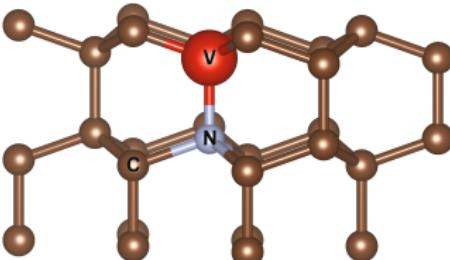
Cubic diamond



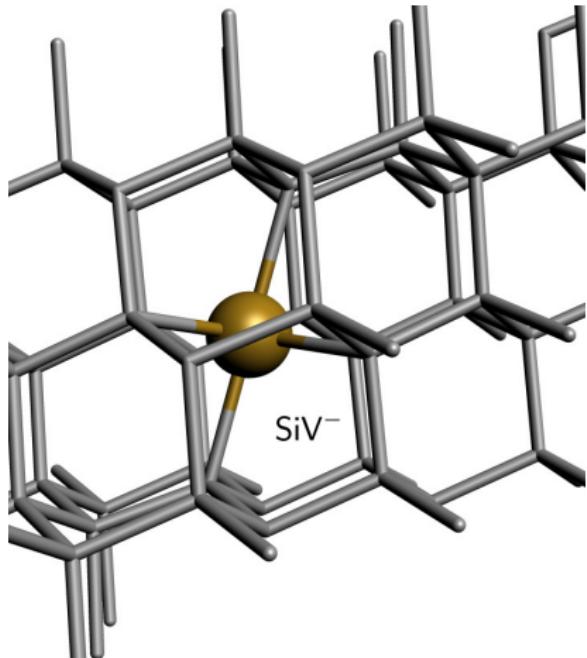
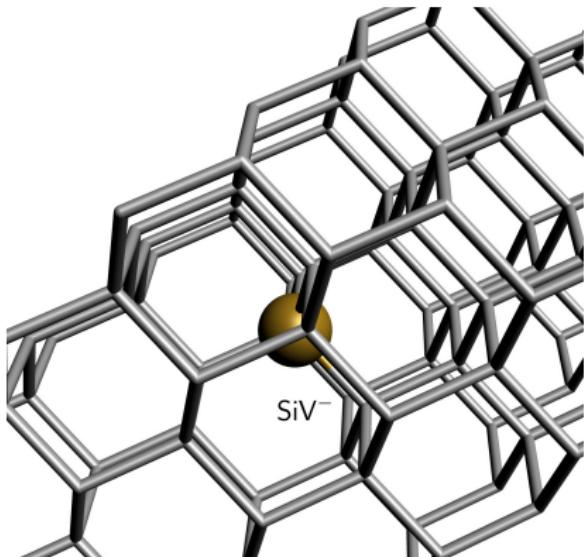
Hexagonal x-type



Hexagonal z-type

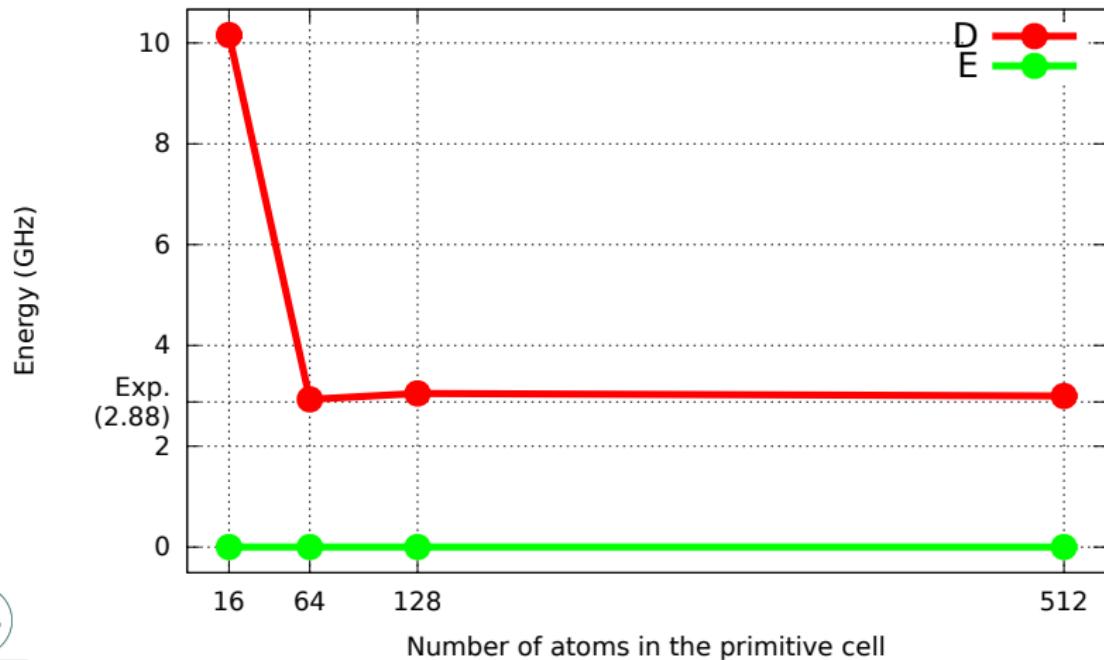


Split vacancies: SiV⁻

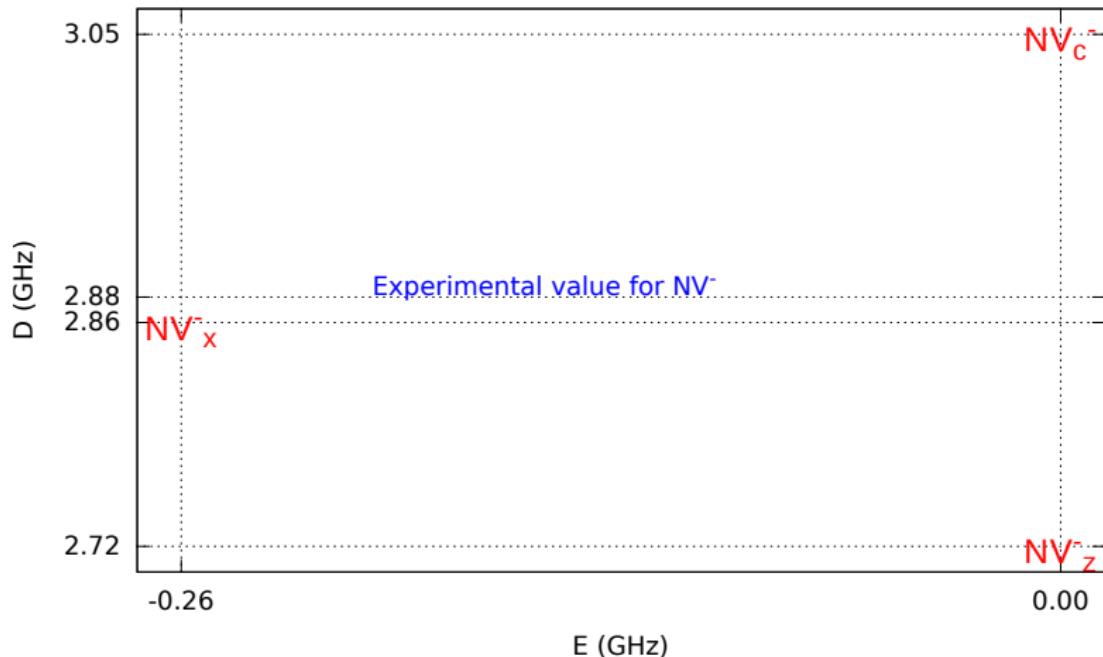


Results

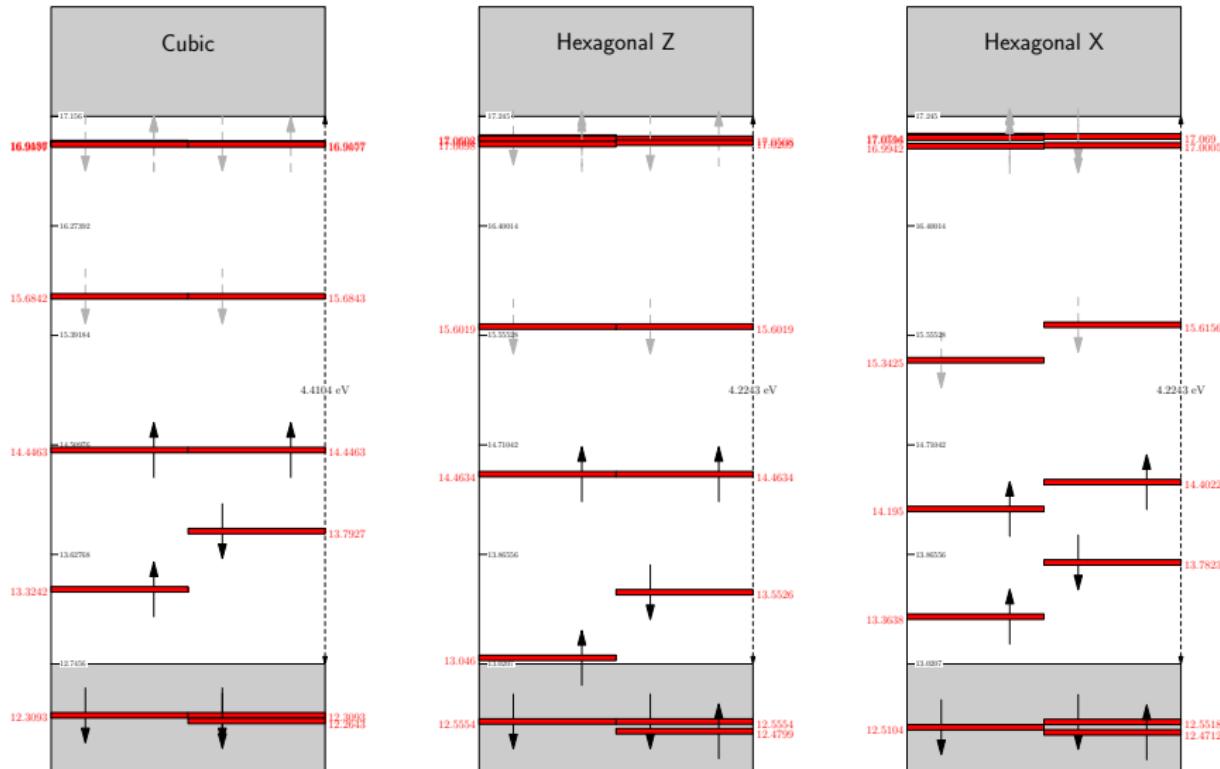
- Cubic diamond, convergence and comparison with the experimental result.



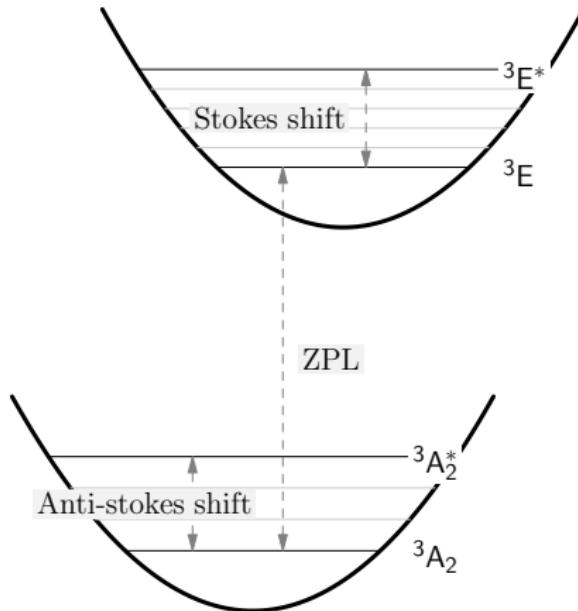
NV*: ZFS cubic (NV_c^*), Hexagonal x, z ($\text{NV}_{x,z}^*$)



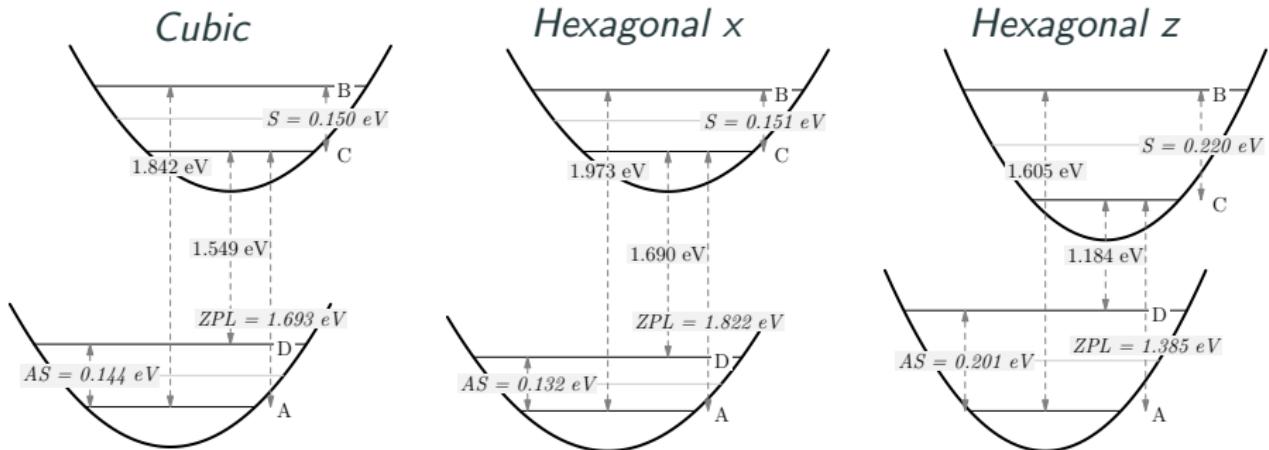
NV⁻: Ground state



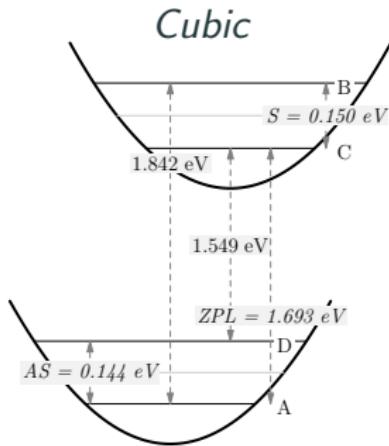
NV⁻: Vibronic scheme (PBE + 128 atomic cell)



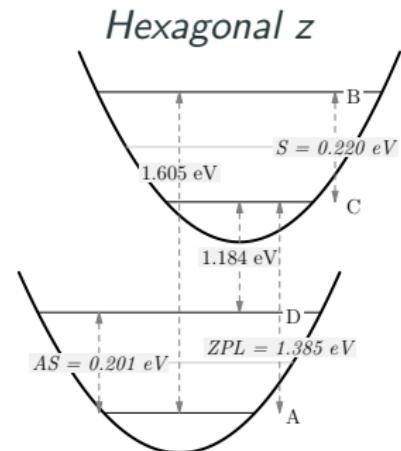
NV⁻: Vibronic scheme (PBE + 128 atomic cell)



NV⁻: Vibronic scheme (PBE + 128 atomic cell)



Experimental data	
ZPL	1.945
$^3A_2 \rightarrow ^3E^*$	2.180
S	0.235
$^3E^* \rightarrow ^3E$	1.760
AS	0.185



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 He
Boron		Carbon		Nitrogen		Oxygen		Flourine		Neon	
Aluminum	26.982	Silicon	28.086	Phosphorus	30.974	Sulphur	32.065	Chlorine	35.453	Argon	39.948
Gallium	69.723	Germanium	72.64	Arsenic	74.922	Selenium	78.96	Bromine	79.904	Krypton	83.8
Indium	114.82	Tin	118.71	Antimony	121.76	Tellurium	127.6	Iodine	126.9	Xenon	131.29
Thallium	204.38	Lead	207.2	Bismuth	208.98	Polonium	209	Astatine	210	Radon	222
Ununtrium	284	Ununquadium	289	Ununpentium	288	Ununhexium	293	Ununseptium	292	Ununoctium	294



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!

