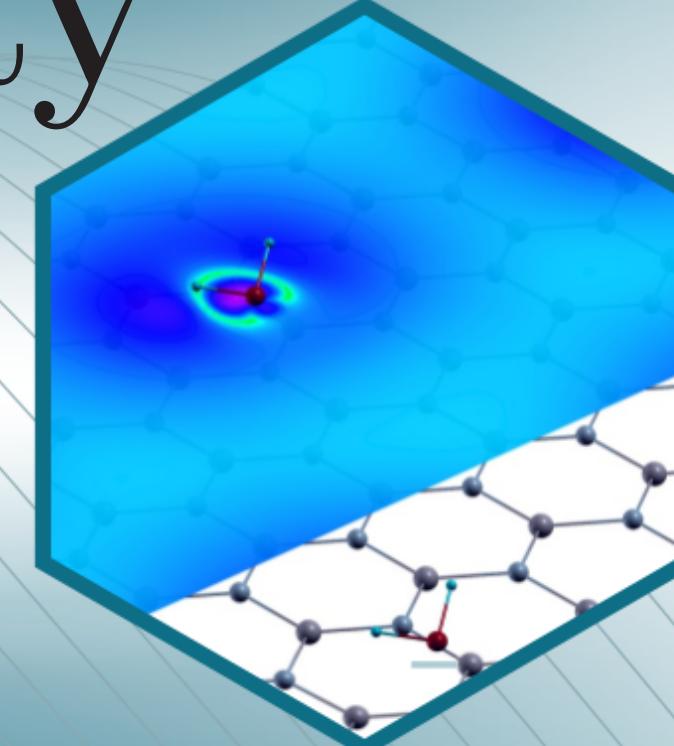




Ab-initio simulations of vacancy-impurity complexes in carbon allotropes

A. Gallo, H. Fedder, T. Gruber, S. Sharma, J. Wrachtrup
and A. Grüneis

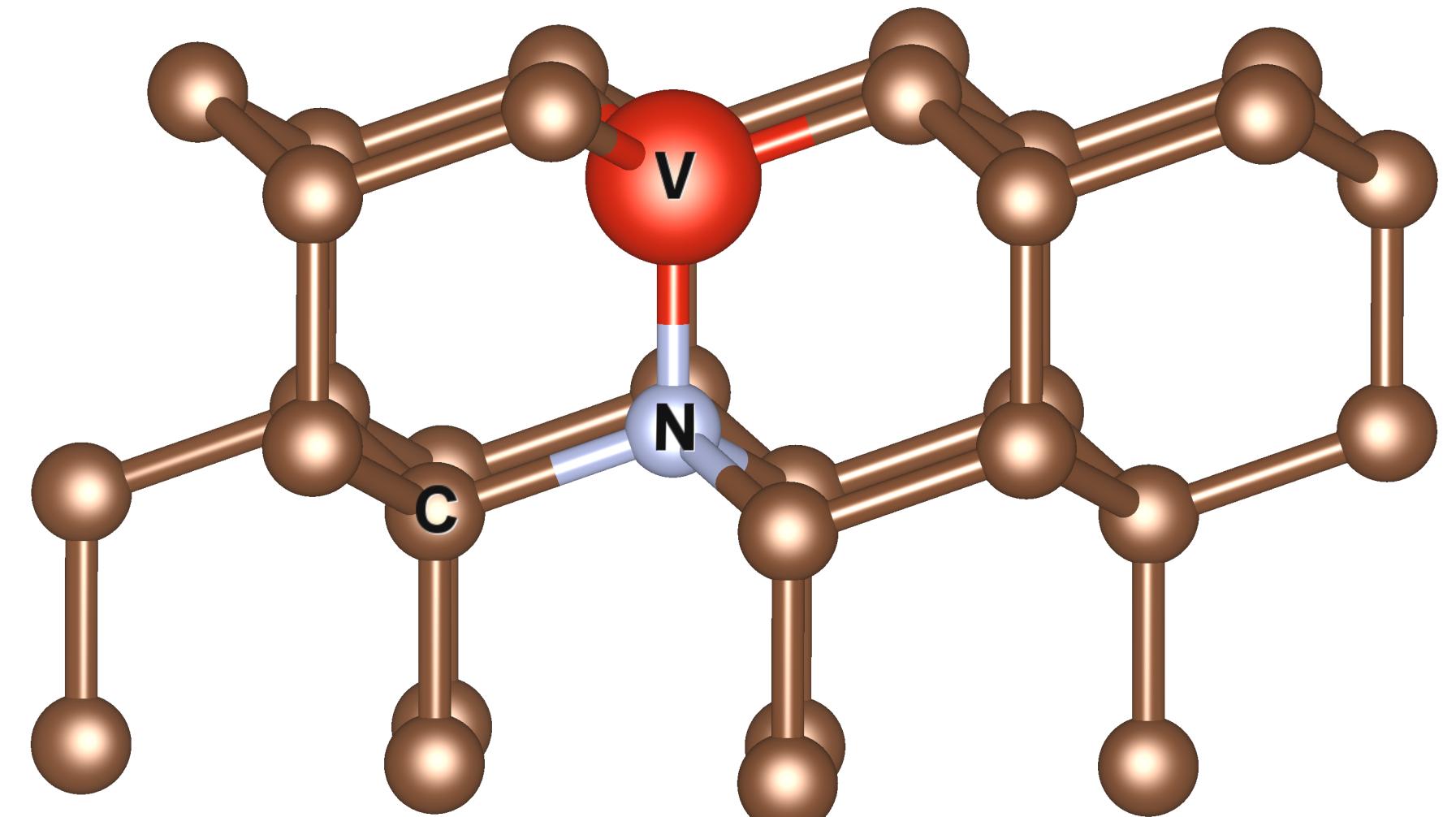


Max-Planck-Institute for Solid State Research, Stuttgart, Germany
a.gallo@fkf.mpg.de

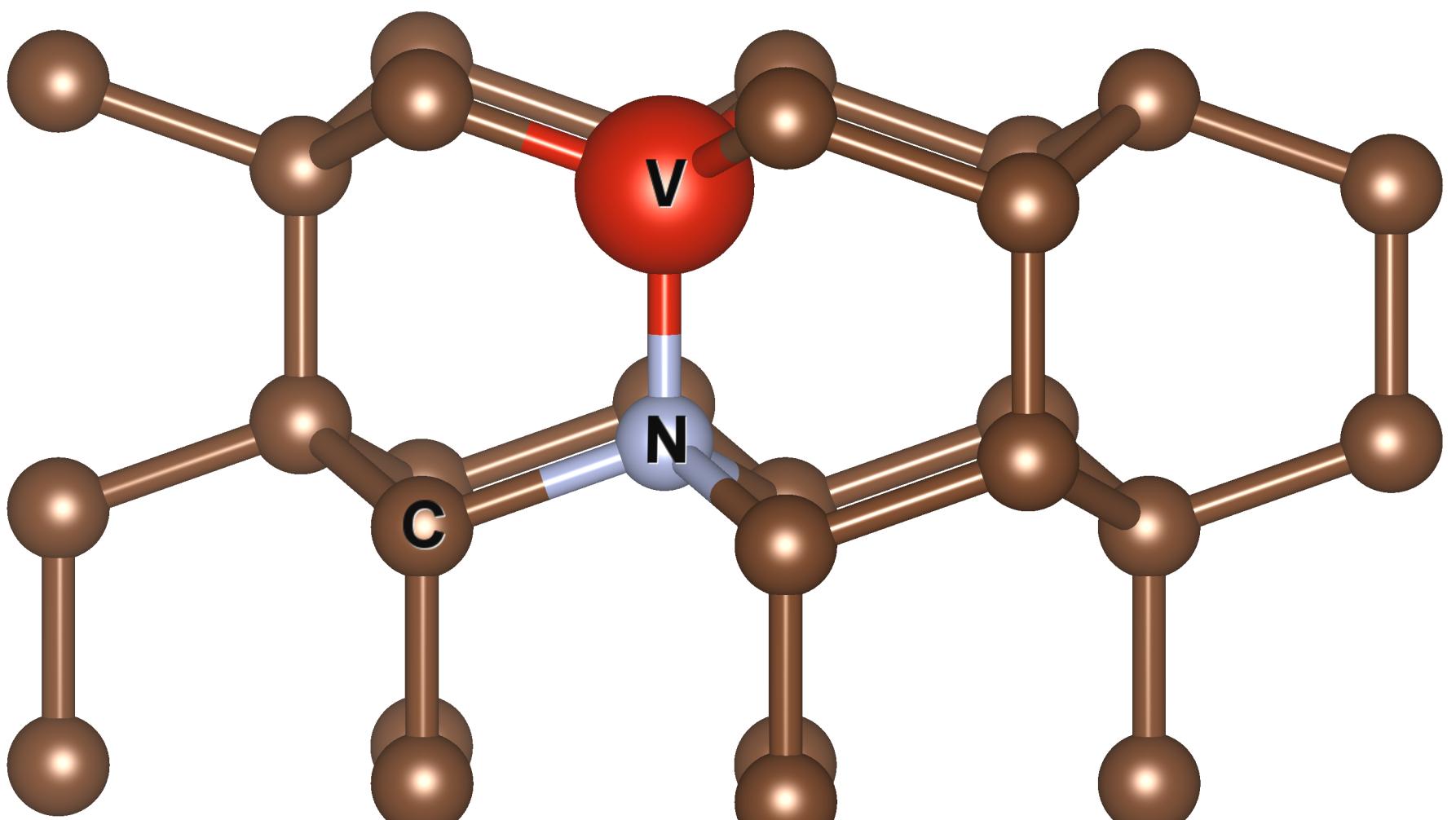
Introduction

Nitrogen Vacancy defects in diamond have become over the last years an important candidate for a bulk room temperature quantum information processing device. In this poster we investigate the feasibility of approximate density functional theory calculations for describing optical and electronic properties for several vacancy-impurity complexes in different carbon allotropes.

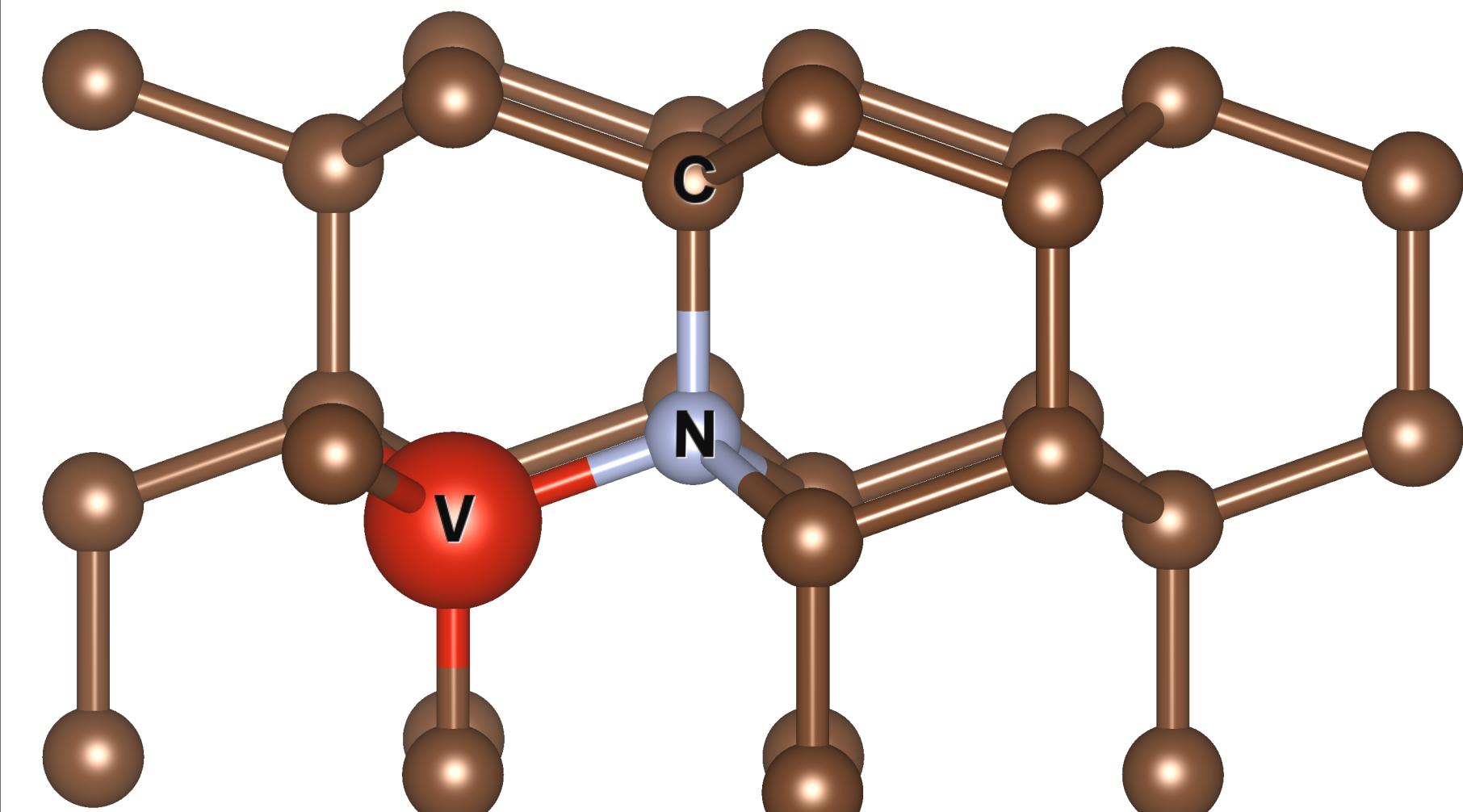
Cubic structure



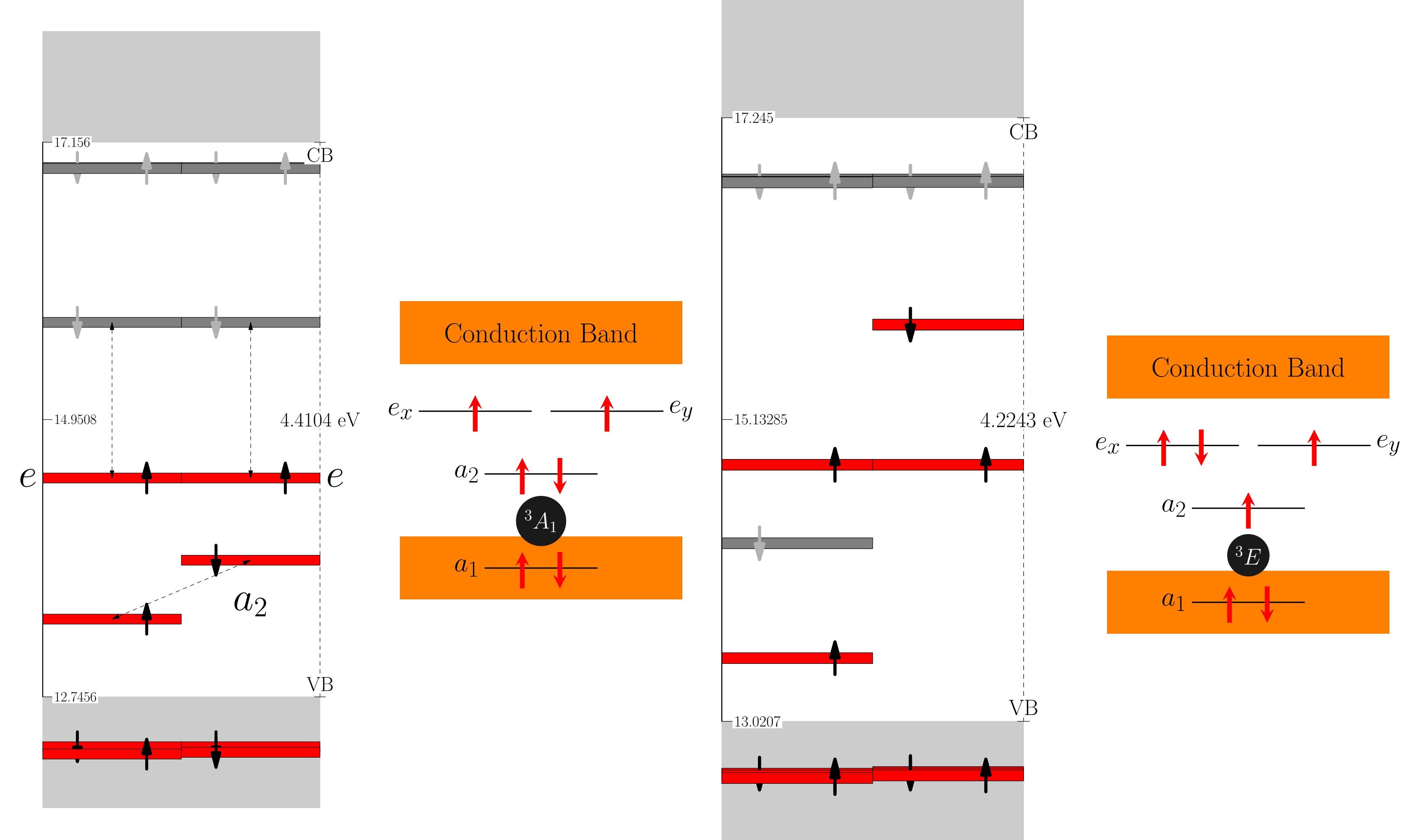
Hexagonal z-type



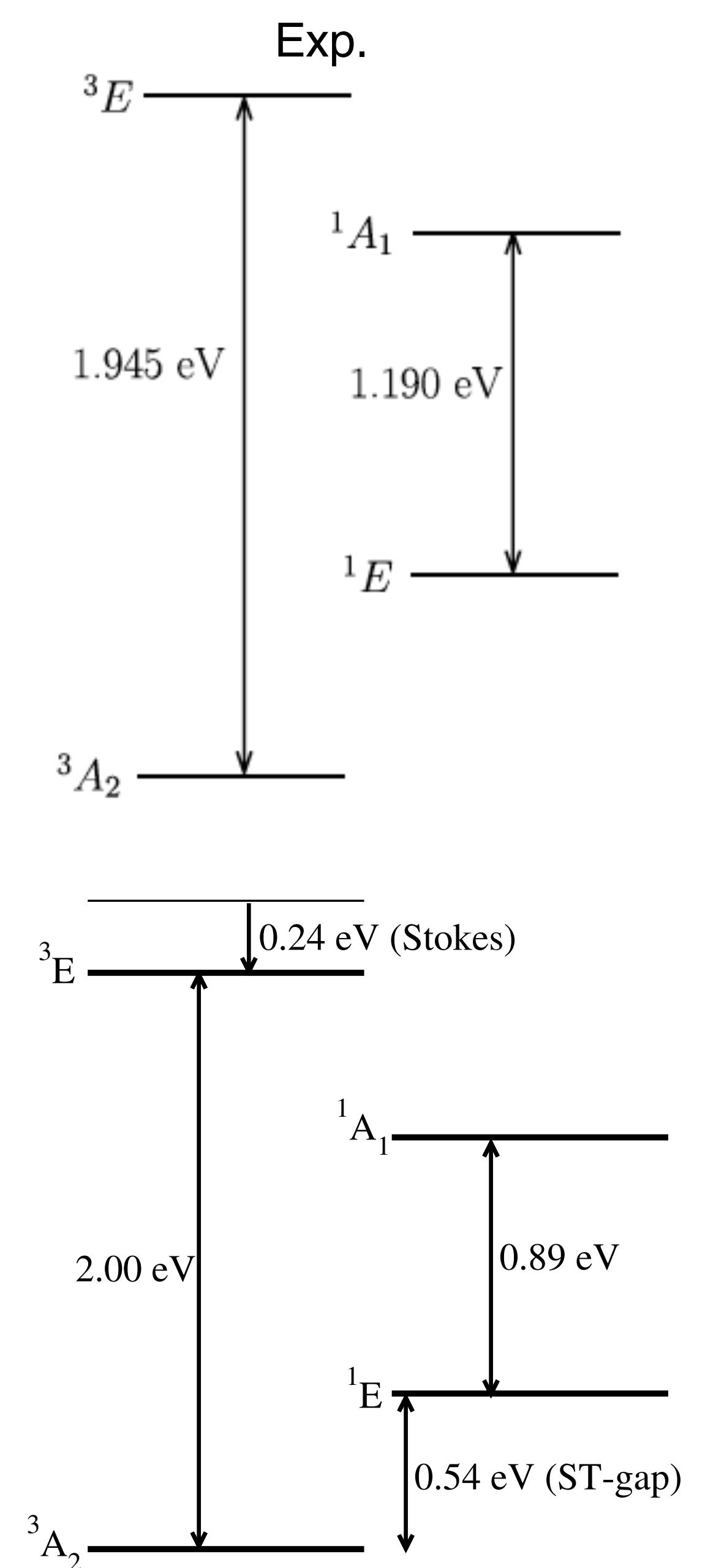
Hexagonal x-type



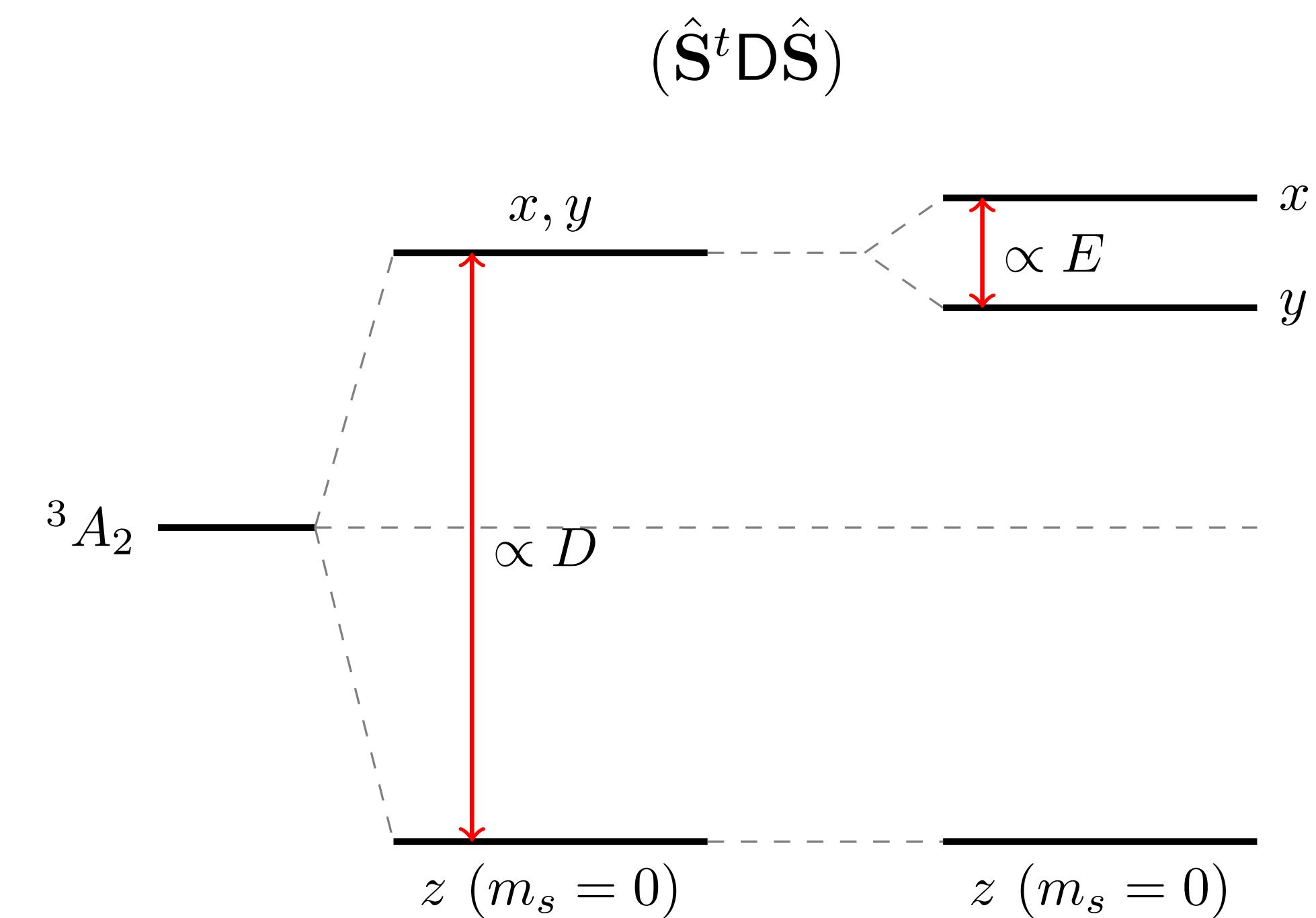
Triplet states 3A_2 and 3E



DMRG calculations



Spin-Spin interaction



$$D = \begin{pmatrix} -E - \frac{1}{3}D & E - \frac{1}{3}D & \frac{2}{3}D \\ & & \end{pmatrix}$$

Type	D (GHz)	E (GHz)
cubic	3.04	0.0
x-type	2.86	-0.25
z-type	2.72	0.0
Exp. [1]	2.88	0

Computational details

- Calculations performed using VASP.
- DMRG calculations done using S. Sharma and G. Chan Block code.
- Plane waves basis set.
- PBE exchange-correlation functional.
- Unit cell size of 128 atoms.
- VASP zero field splitting implementation.

Discussion

- Prediction of new types of defects by studying diamond allotropes with and negatively charged NV center as a test case.
- Calculation of defect fingerprints such as the spin-spin interaction parameters E and D .
- Calculation of NV⁻ excited states self-consistently by interfacing VASP with Block.