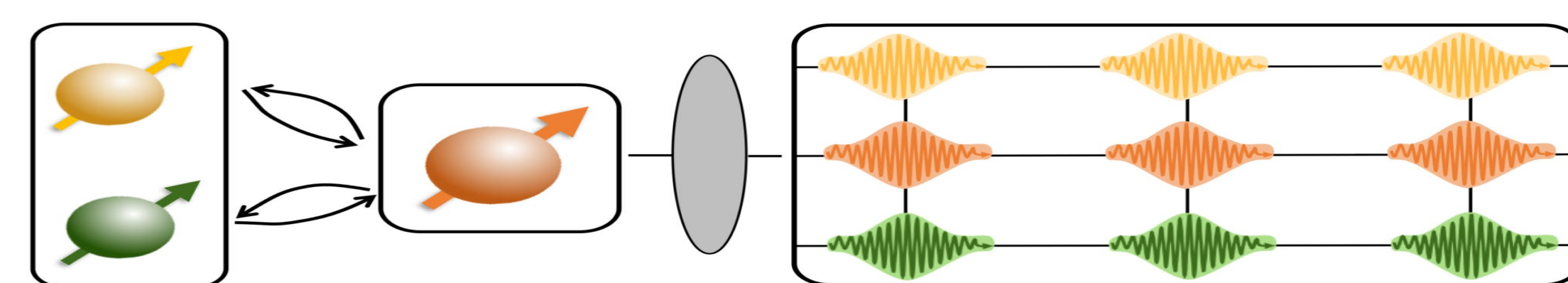
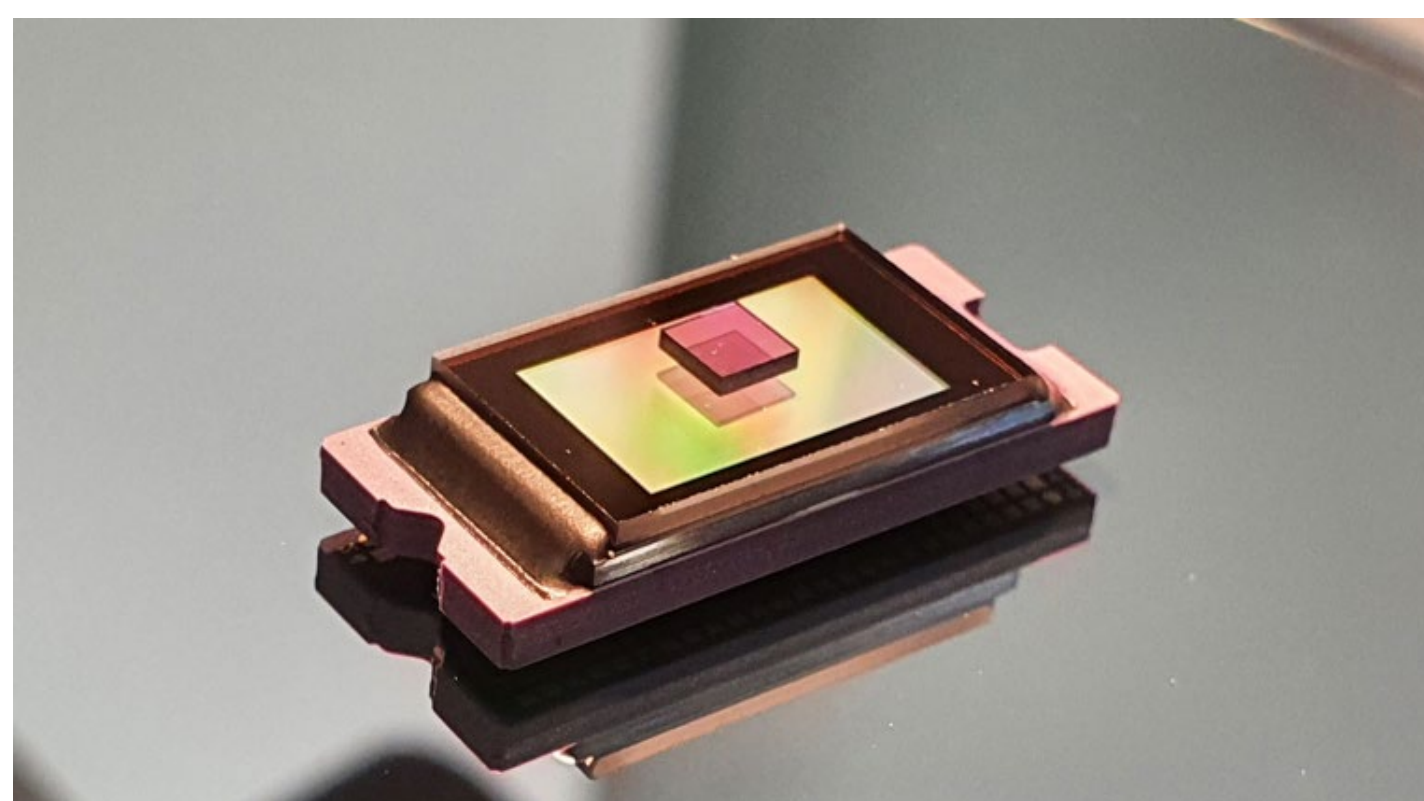
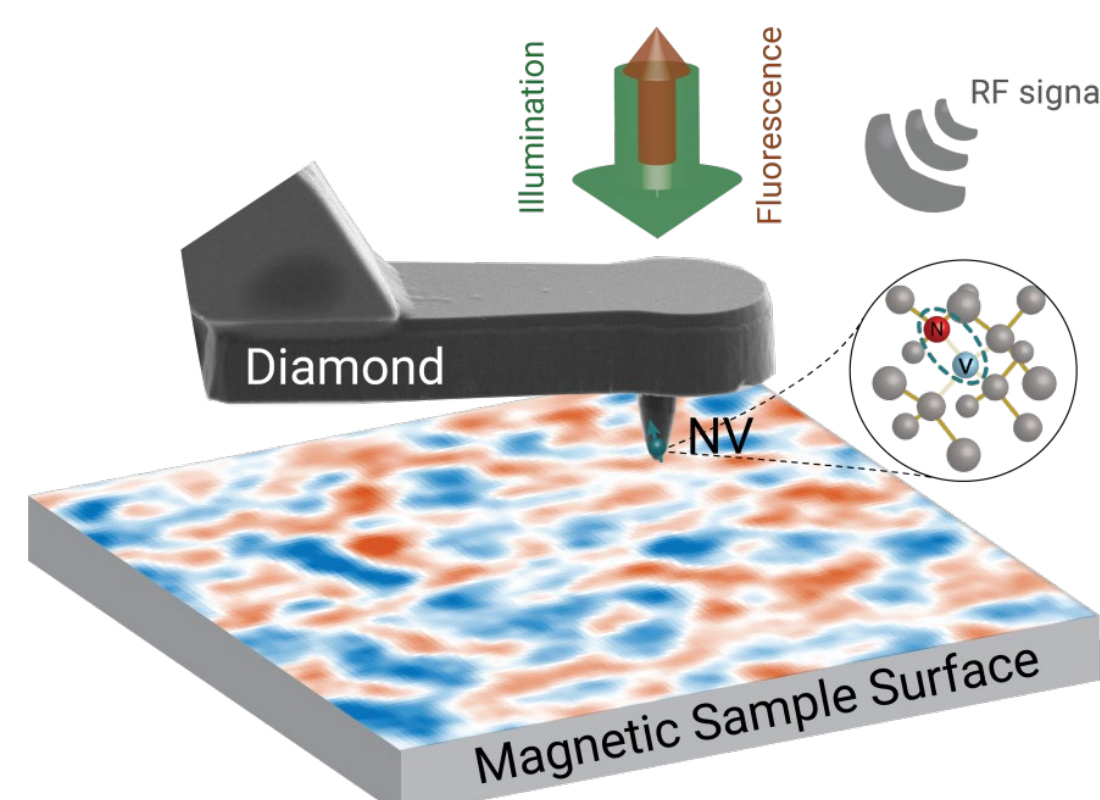


Wigner 121 Scientific Symposium

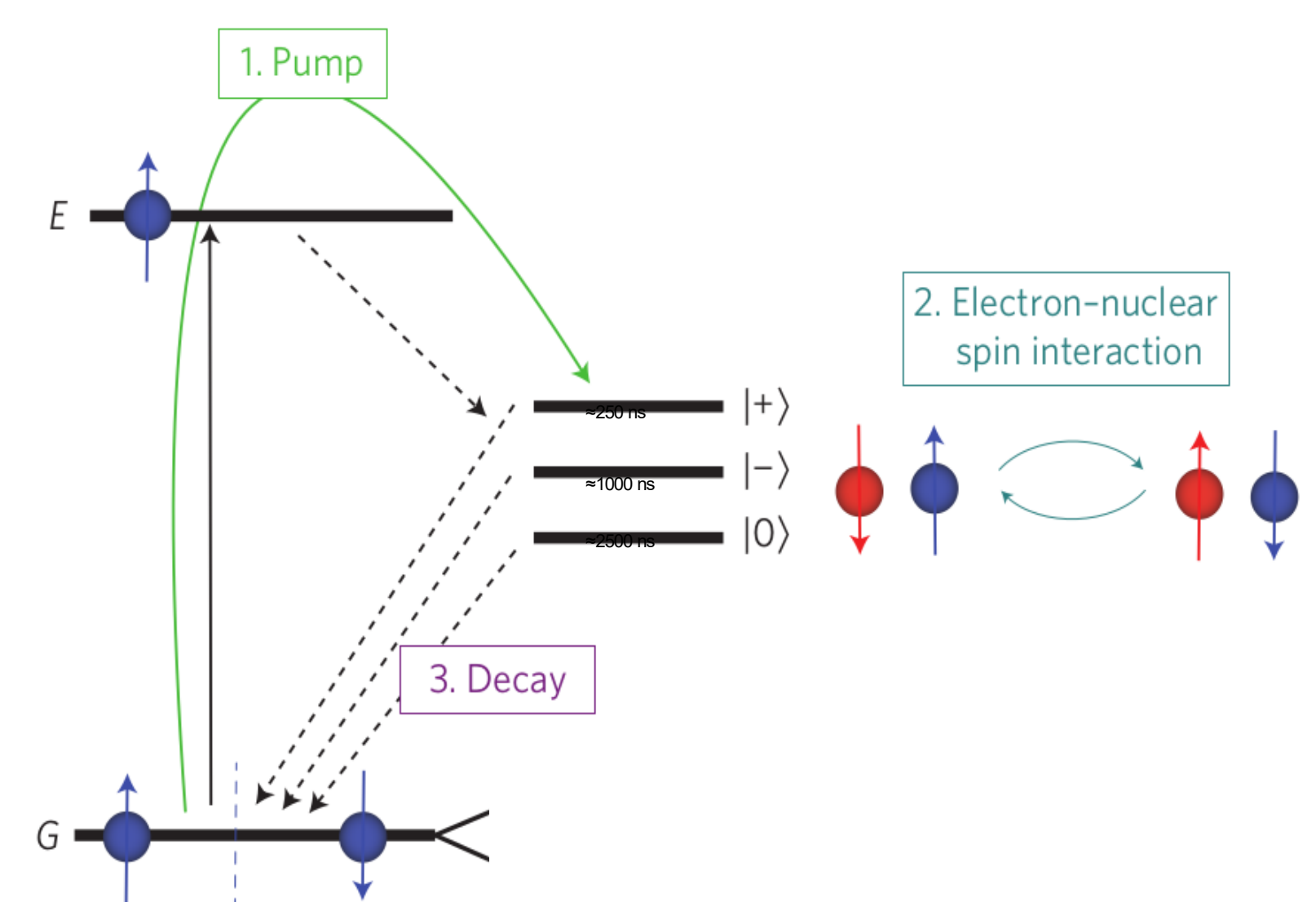
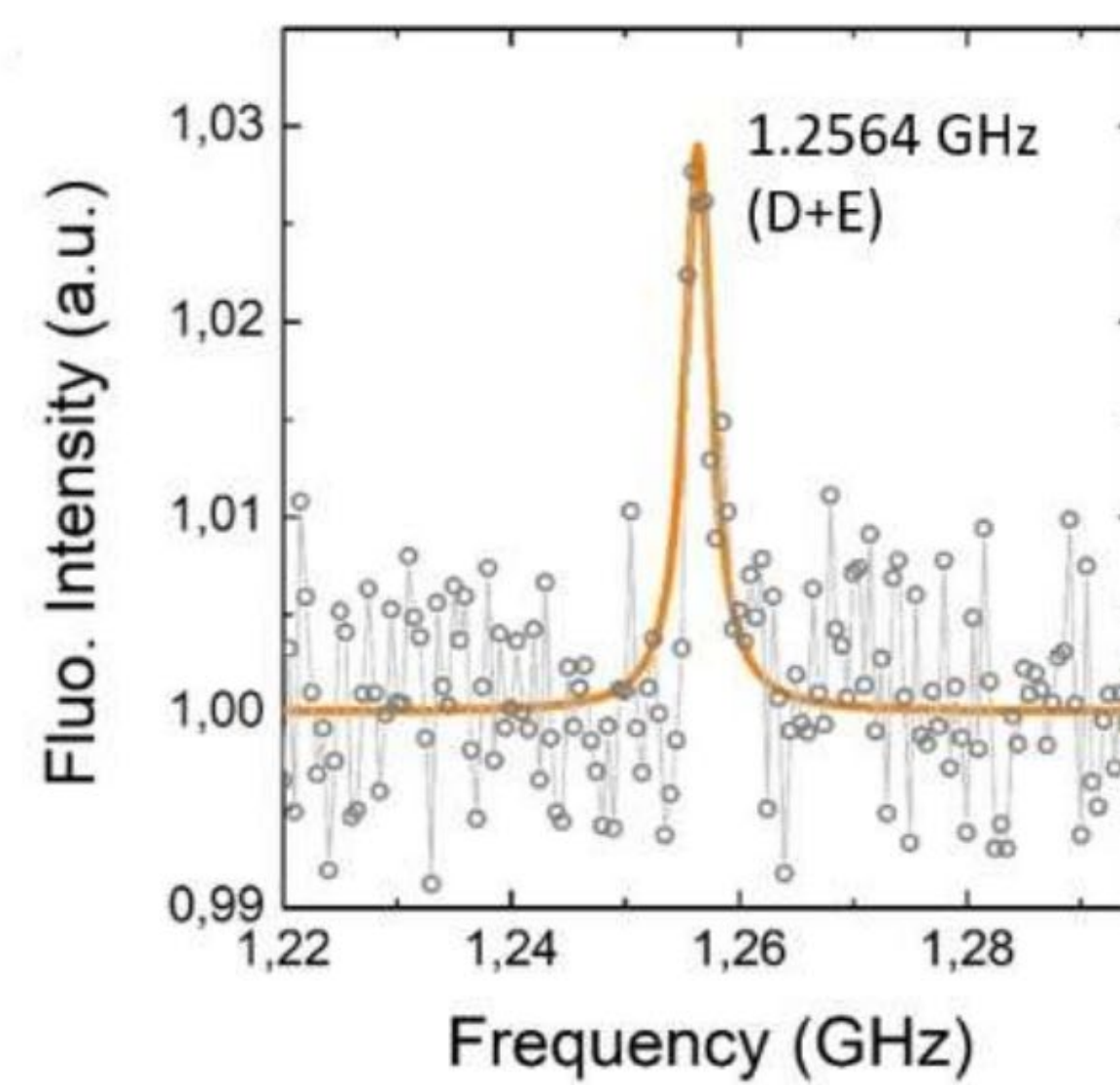
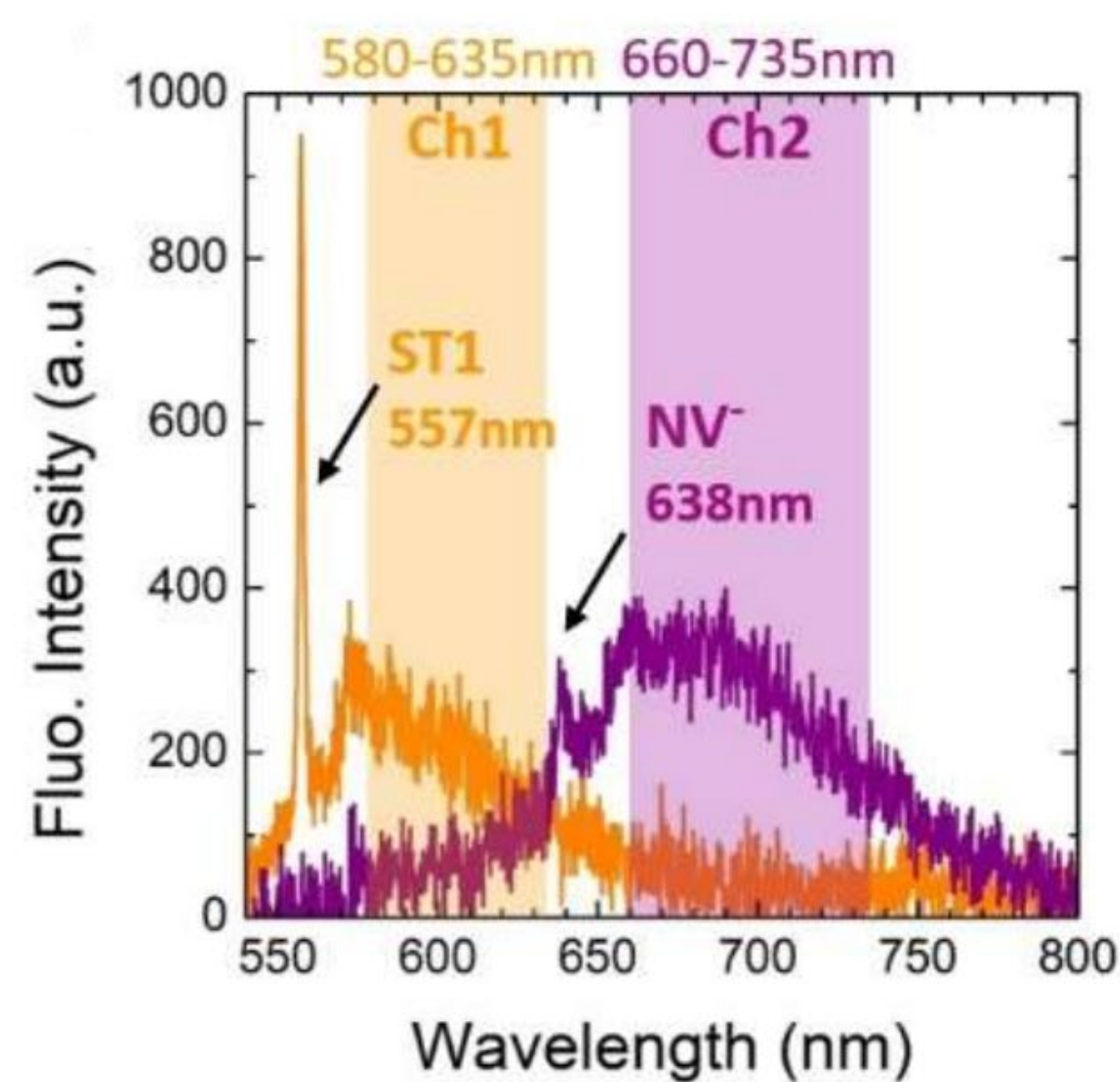
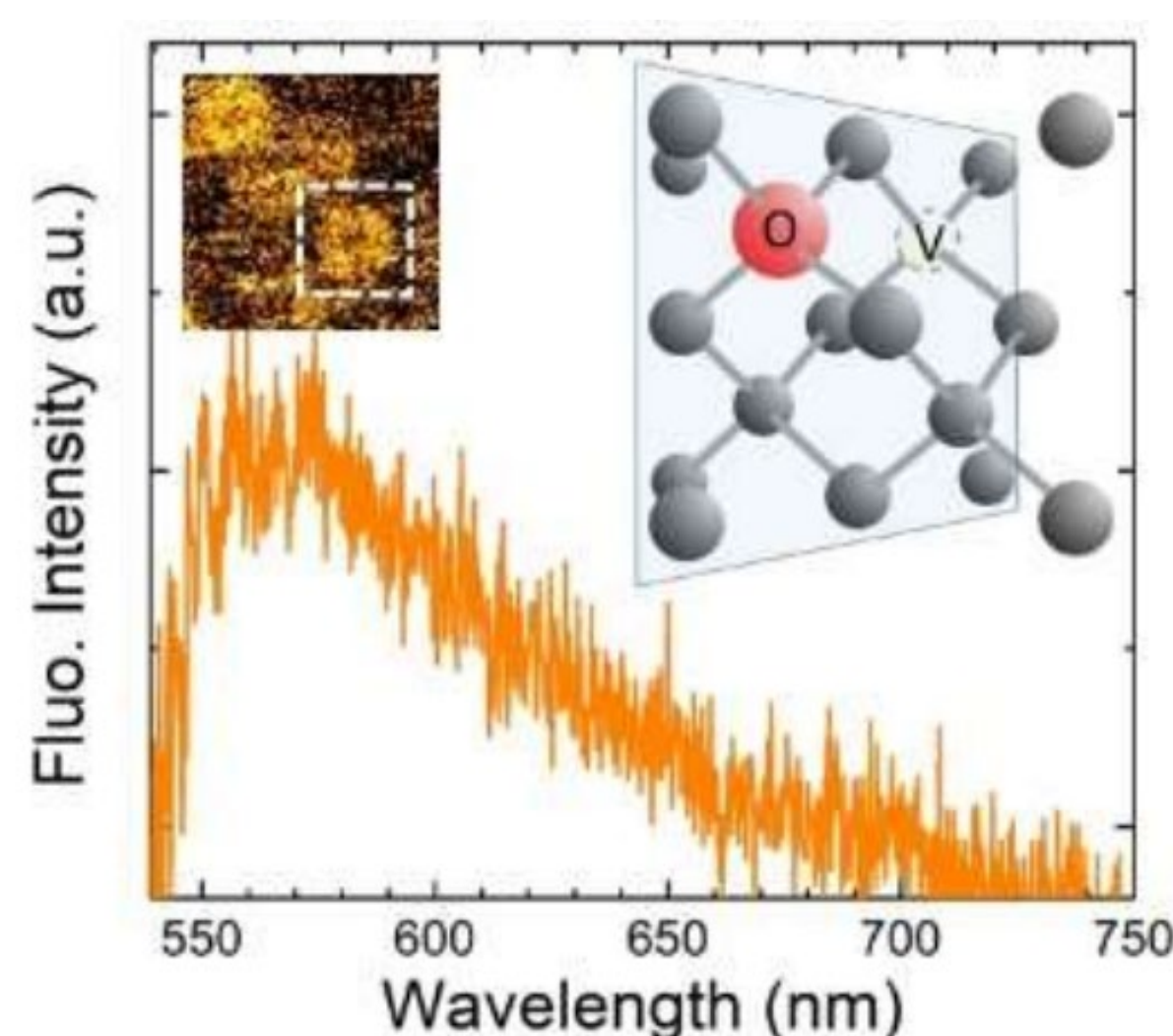
Wigner Research Centre for Physics
Institute of Solid State Physics and Optics
Department of Theoretical Solid State Physics
Semiconductor Nanostructures Research Group

Introduction

Diamond quantum technologies are widespread in different areas of knowledge; like quantum sensing, quantum computing, and quantum communications.

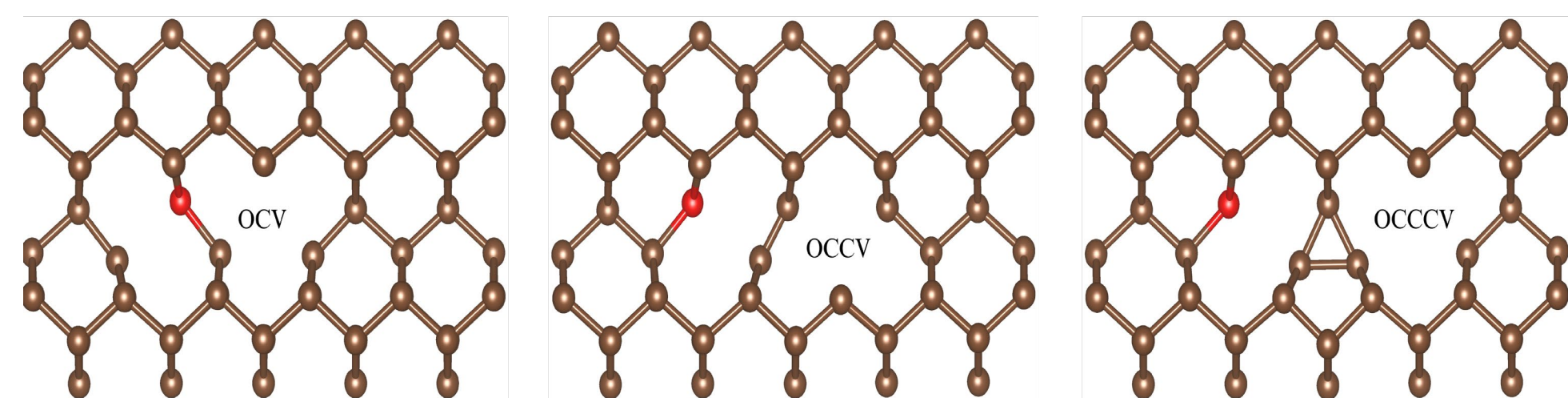


ST1 color center is a single photon emitter which was discovered in diamond nanowire. This center in diamond can be a long-living solid-state quantum memory. There was a hint from experiments to verify this oxygen-vacancy complexes with ab-initio calculations.



Method

- Defects are modeled in supercell contain 512 carbon atoms using vacancy and oxygen substitution along [110] plane.
- We use semilocal PBE and HSE06 hybrid functional.
- We calculated the singlet and triplet spin state. The ZFS calculated.
- 370 eV plane-wave cutoff energy.



Publications of the group

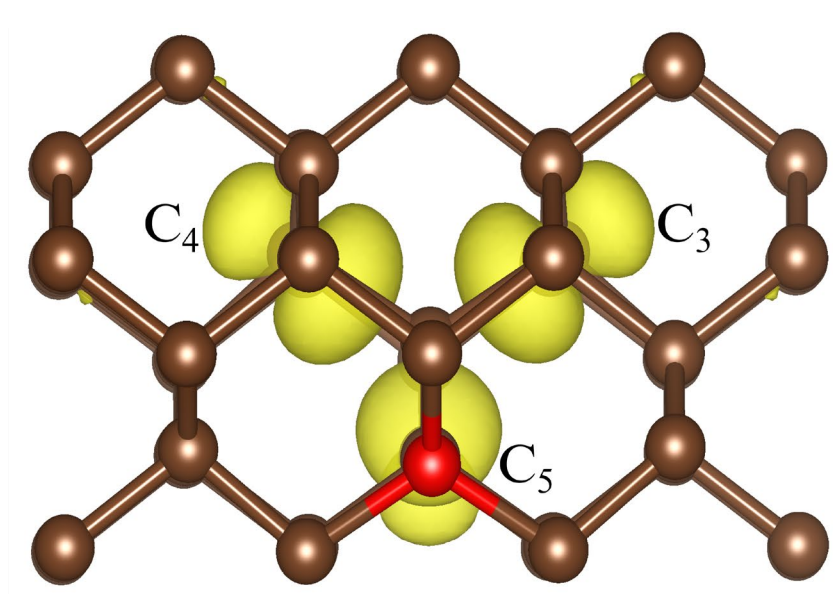
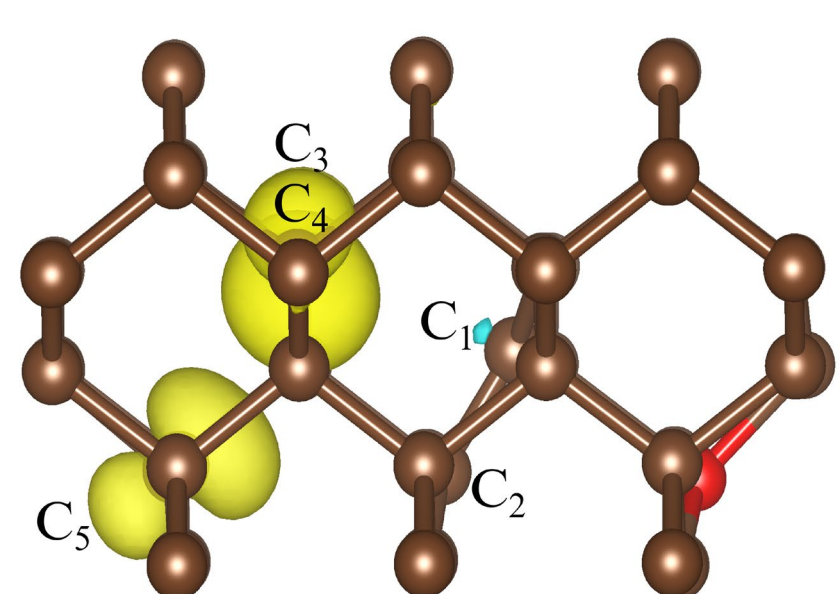
Nima Ghafari Cherati et al 2023
J. Phys.: Condens. Matter 35 315502

Thiering G and Gali A 2016 Phys. Rev. B 94 125202

<https://scholar.google.com/citations?user=1aWvI5wAAAAJ&hl=en>

Results

We found the oxygen-vacancy complexes have a high-spin $S = 1$ ground state. The OCCV complex is a metastable defect that may occur in oxygen doped diamond. The OCCV complex is a near-infrared color center with specific ZFS and hyperfine constants that might be observed in photoluminescence and ESR techniques in oxygen doped diamond



Defect	E_f (eV)	GS	Symmetry	D (MHz)	E (MHz)
ST1 (exp.)	-	S	C_{2v} or lower	1139	135
WAR5 (exp.)	-	T	C_{3v}	2888	0
OV	7.79	T	C_{3v}	2989	0
OCCV	13.35	T	C_{1h}	2886	160
OCCCV	11.93	T	C_{1h}	2771	433
OCCCV	12.51	T	C_{1h}	2929	44

