Modelling of the Photoelectrical Response of NV diamond

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Technical Computing Camp 2026
Brno, Czech Republic

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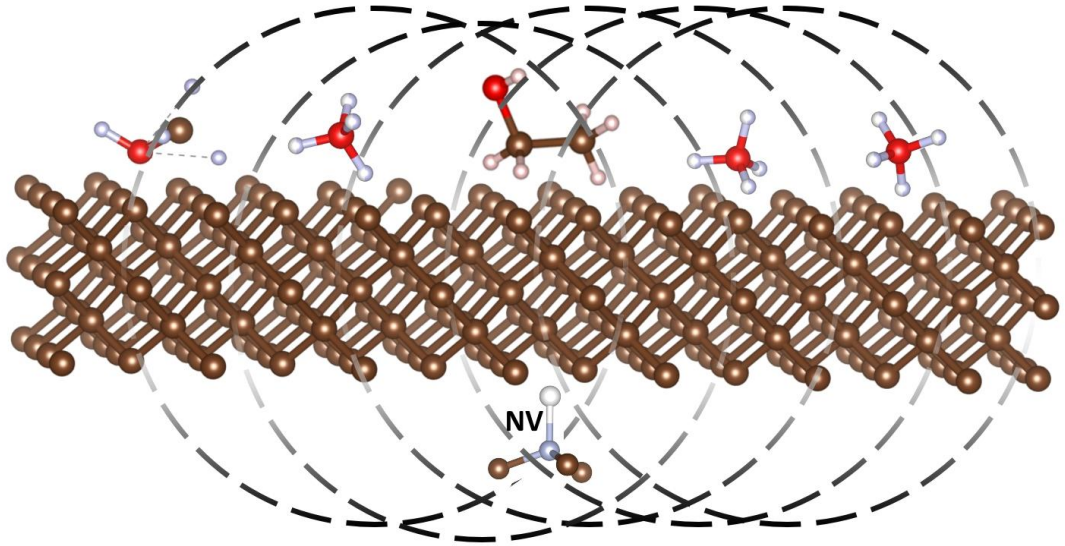
the European Union

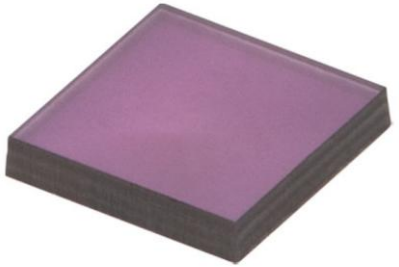
Elementary research on quantum response in fluorescence/photocurrent spectra of physical fields



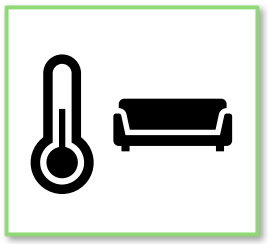
NV defect

Point defect in the crystal latice of the diamond

Complex of the nitrogen atom with a vacancy



Diamond sample with 4.5ppm of NV defects



Working in room temperature

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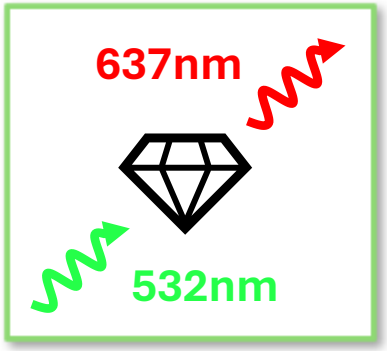
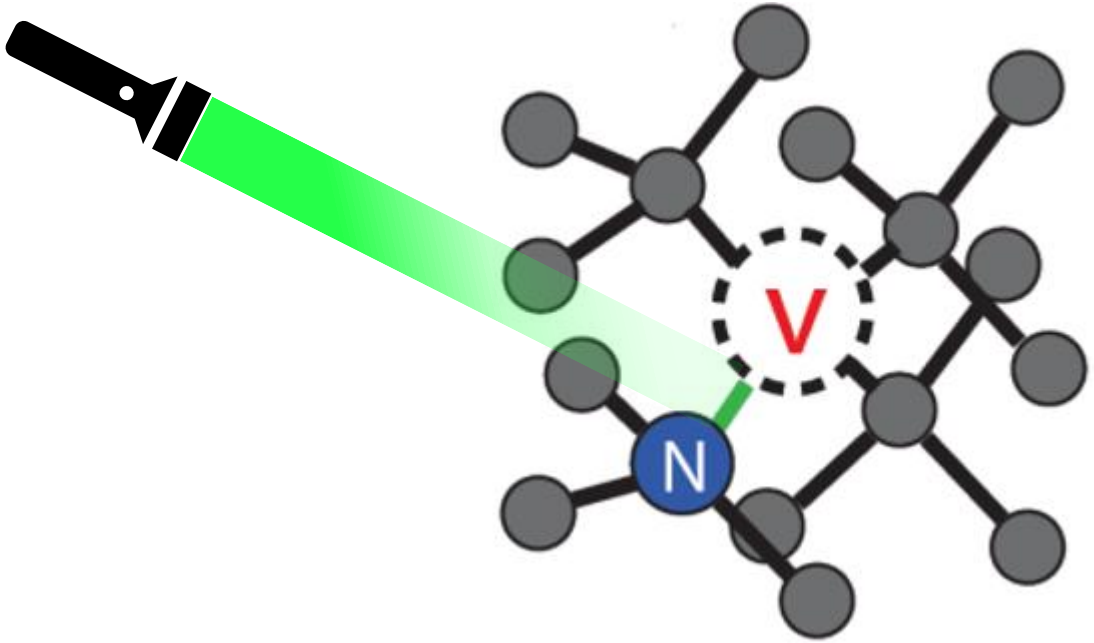
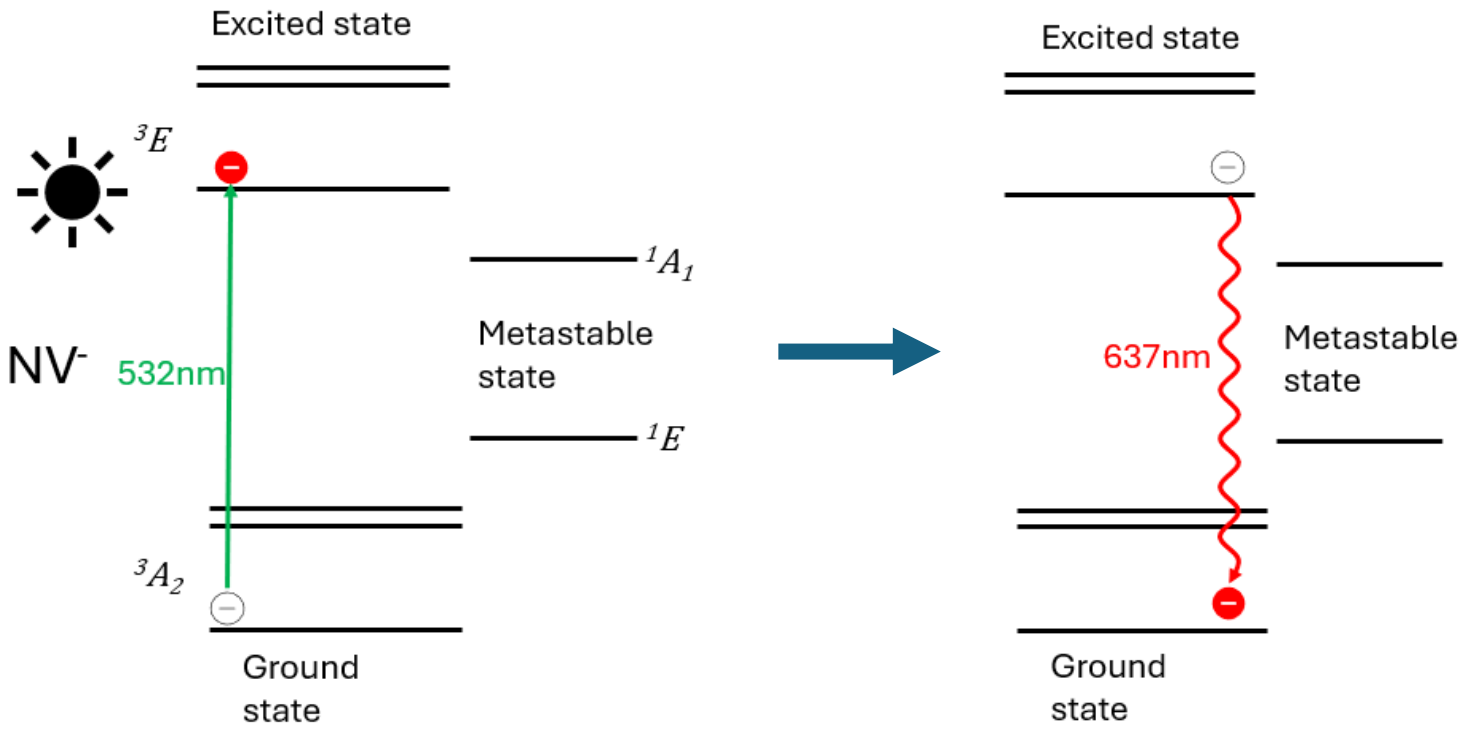


Fluorescence





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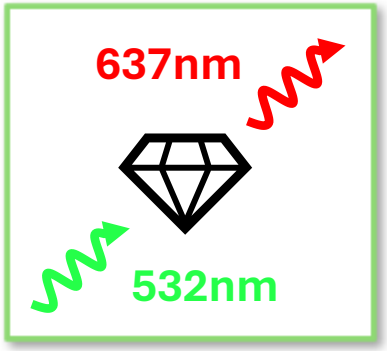
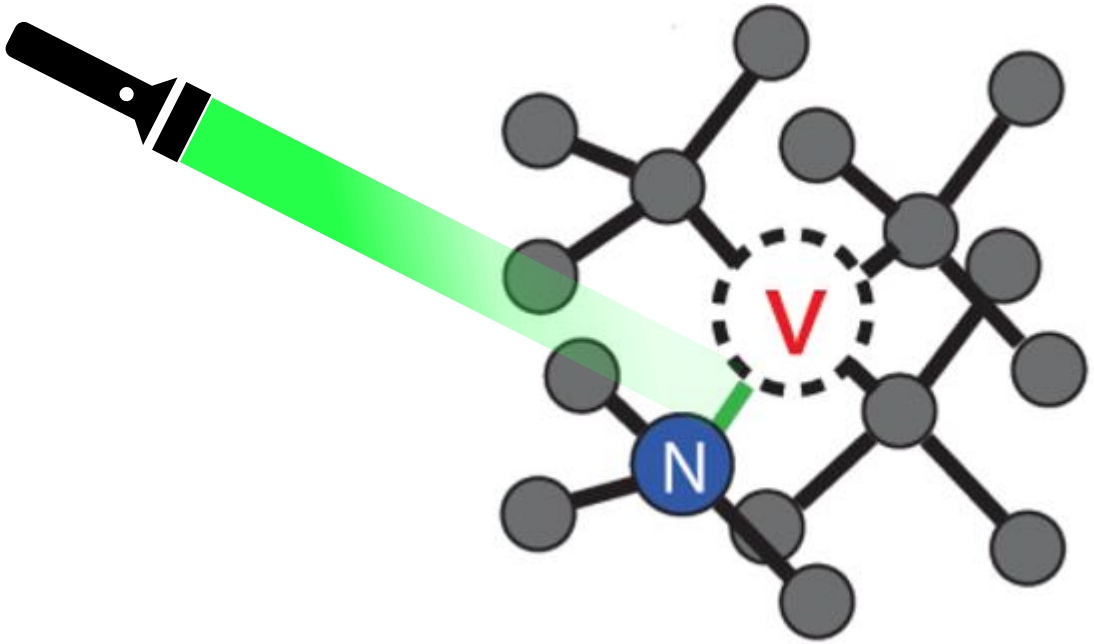
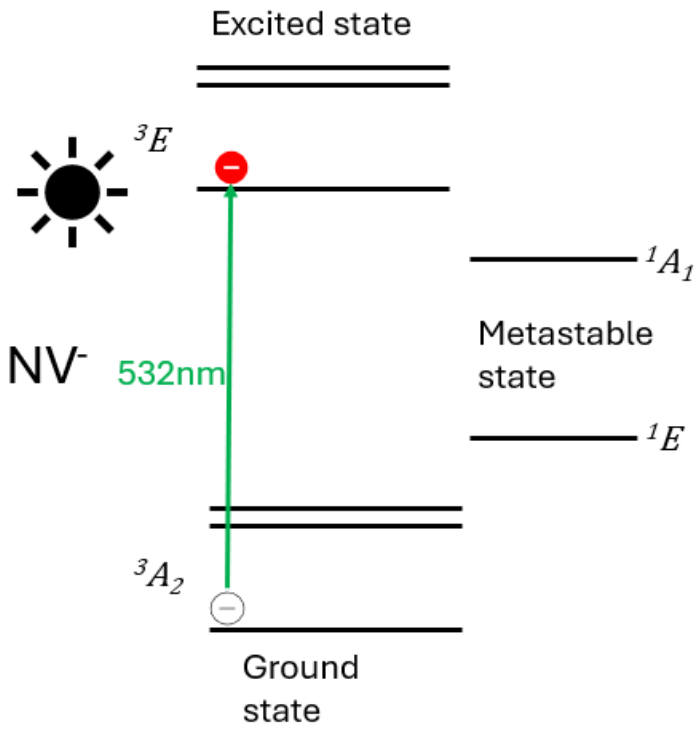
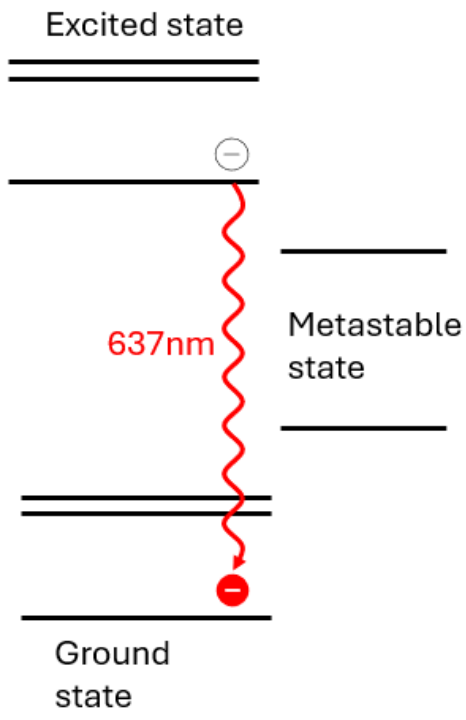
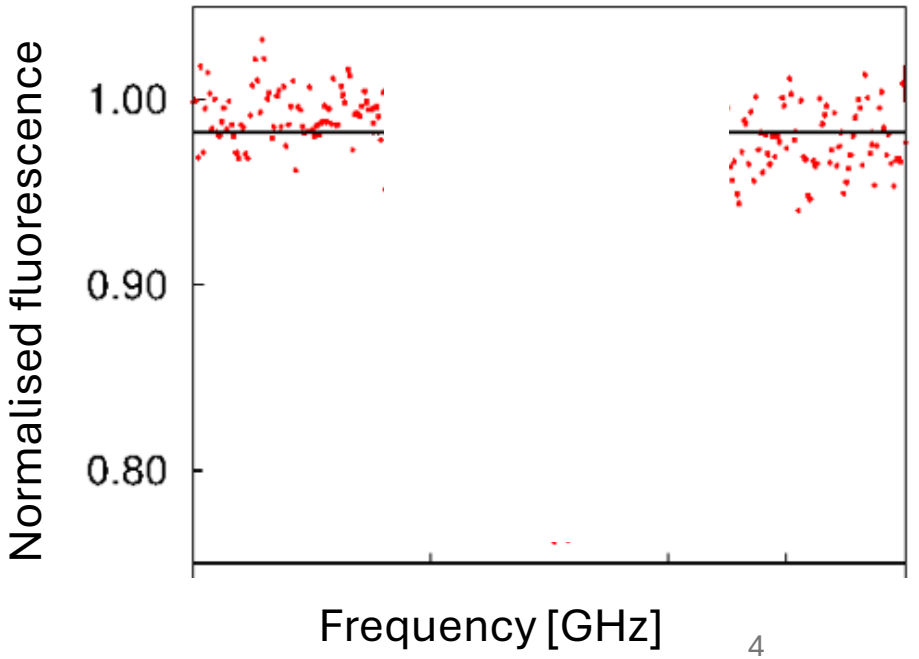


Fluorescence









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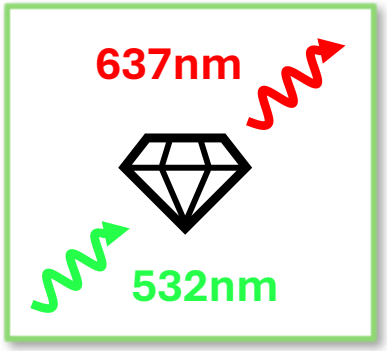
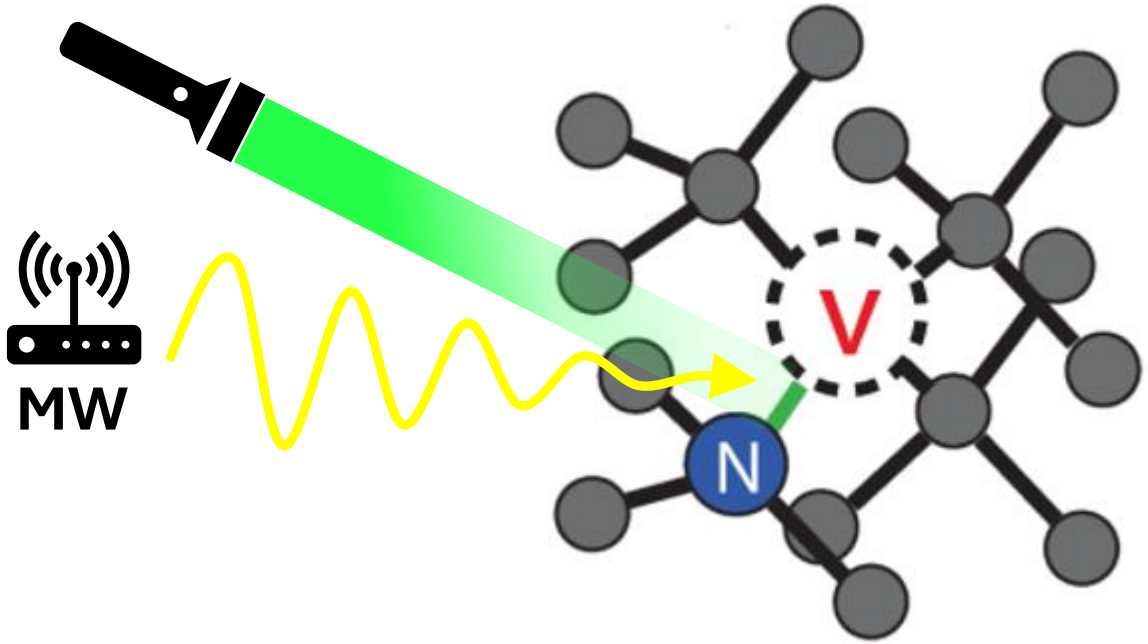
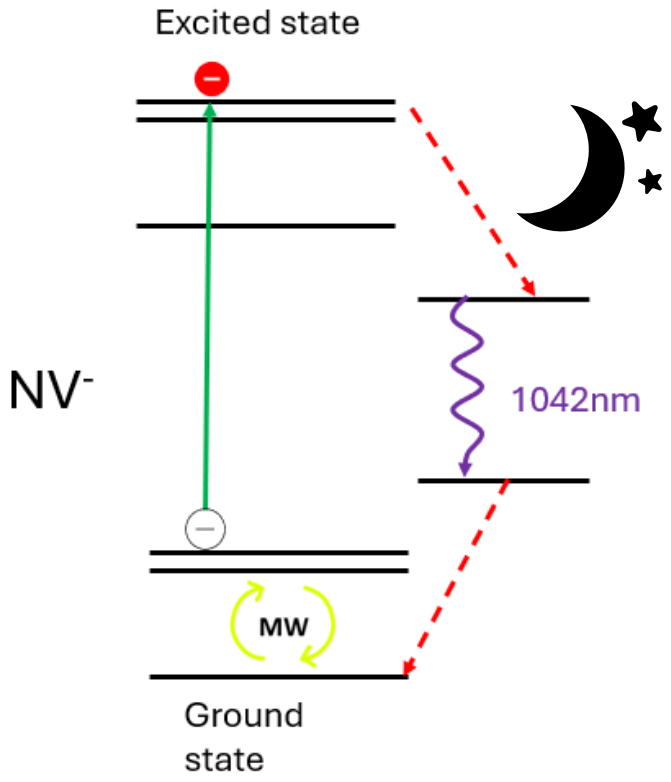
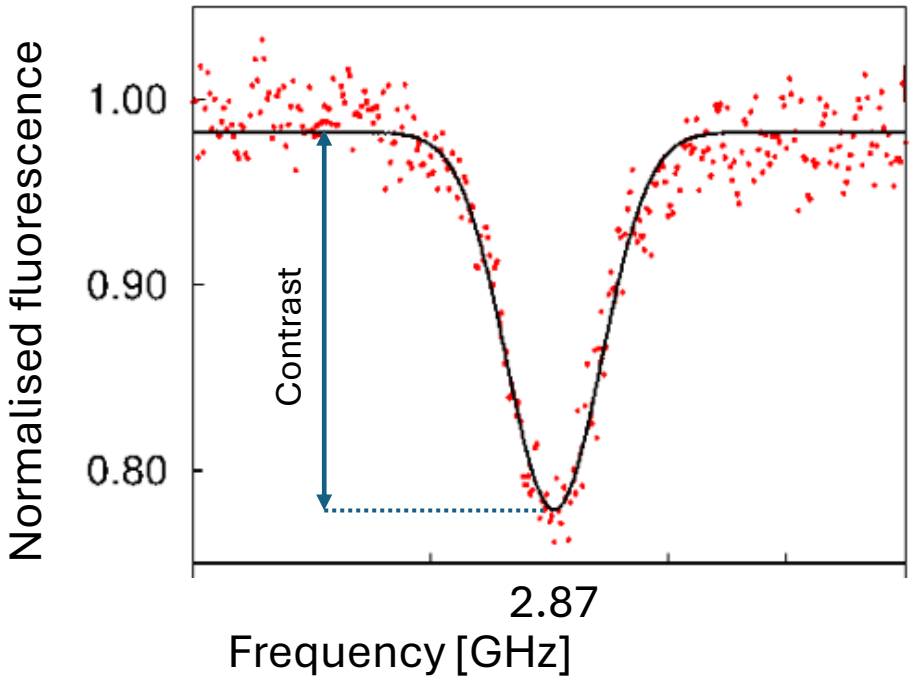


Fluorescence – ODMR[1]





$$C = \frac{I_{off} - I_{on}}{I_{off}}$$



[1] A. Gruber et al. Science 1997

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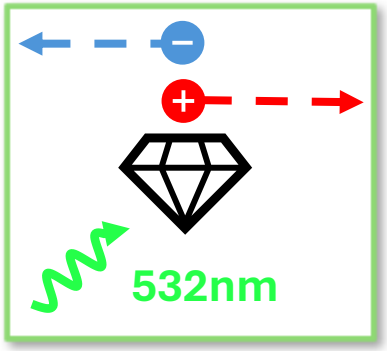
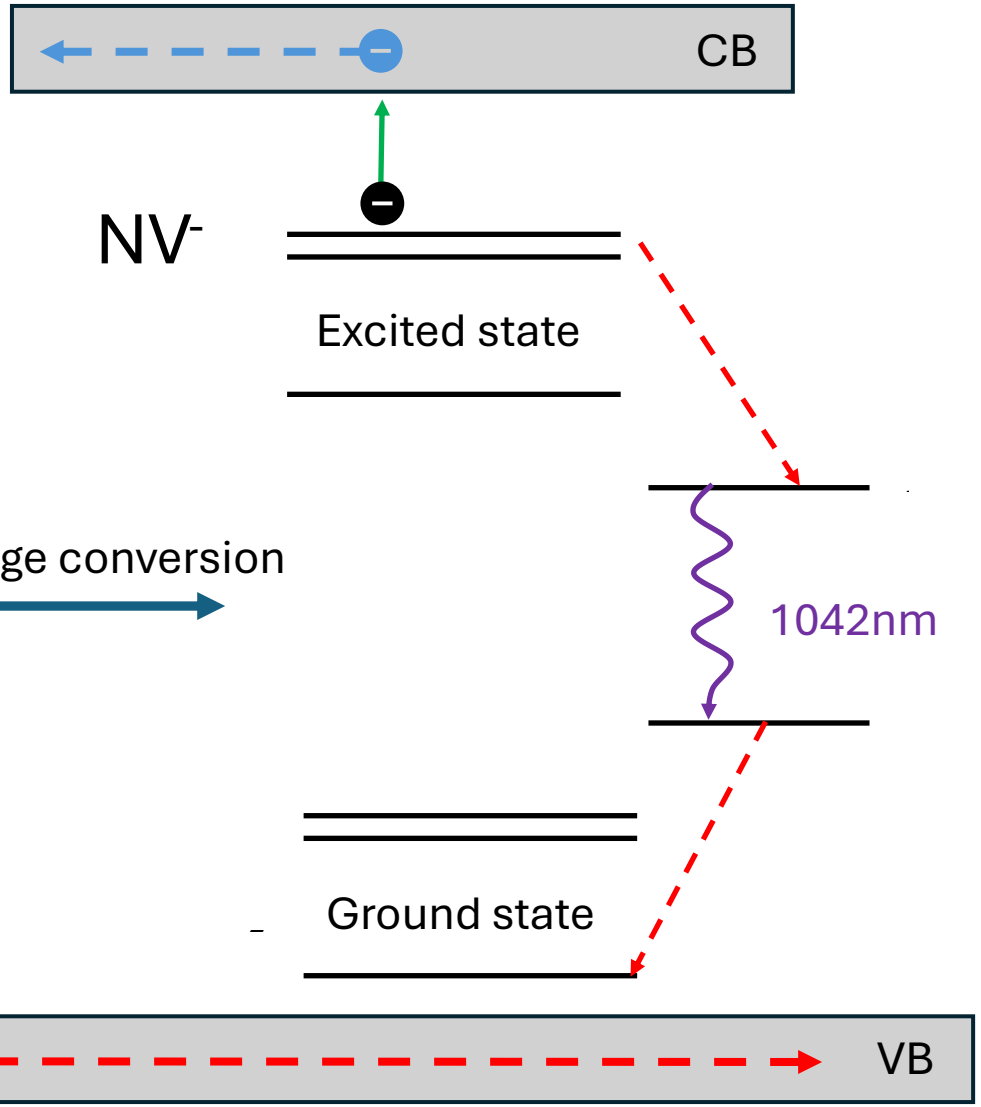
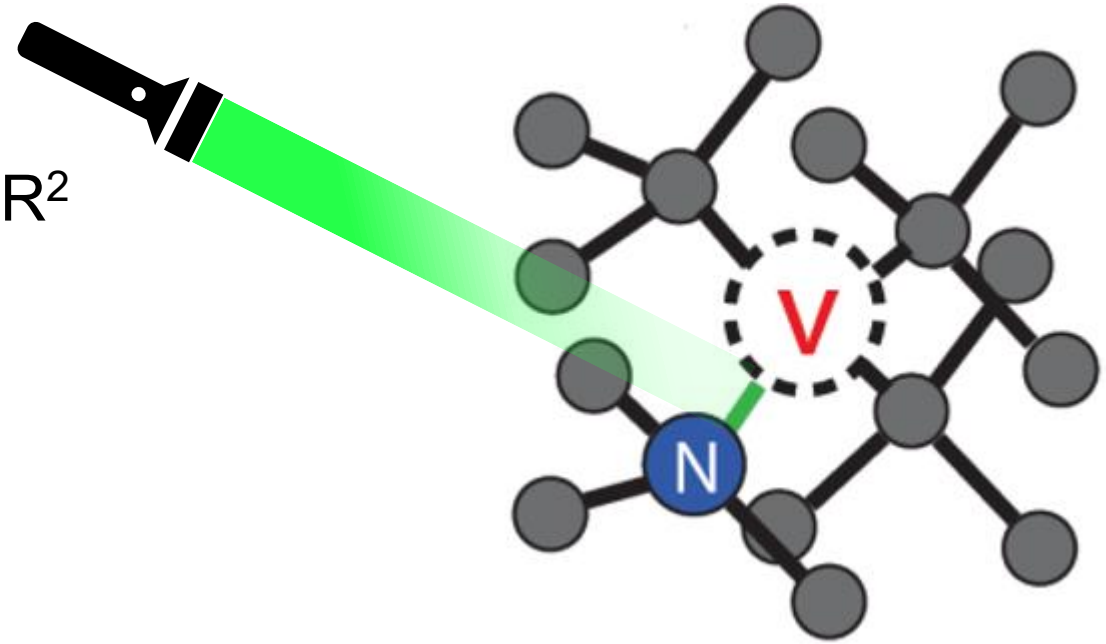
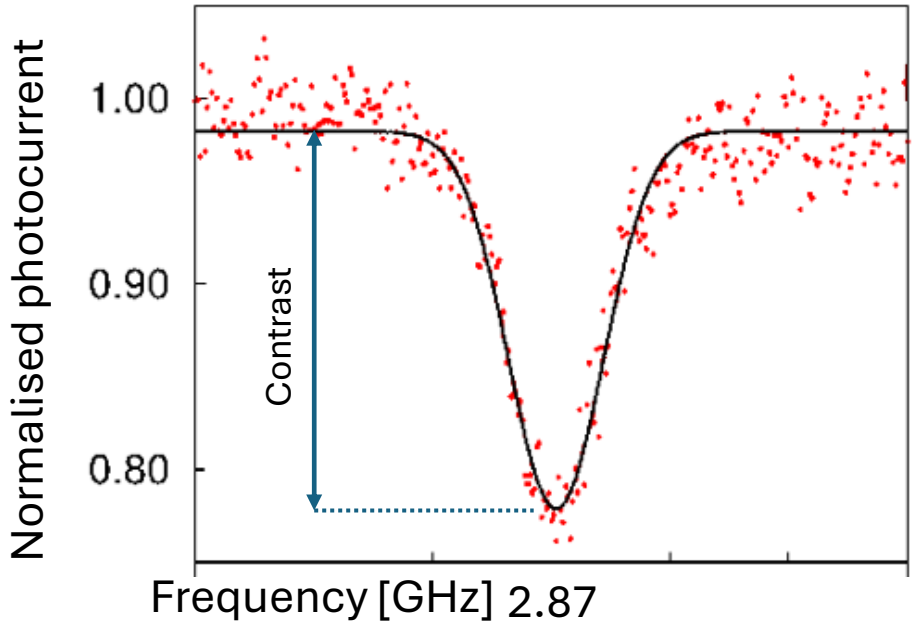


Photocurrent generation – PDMR[2]







2) E. Bourgeois et al., ncomms, 2015

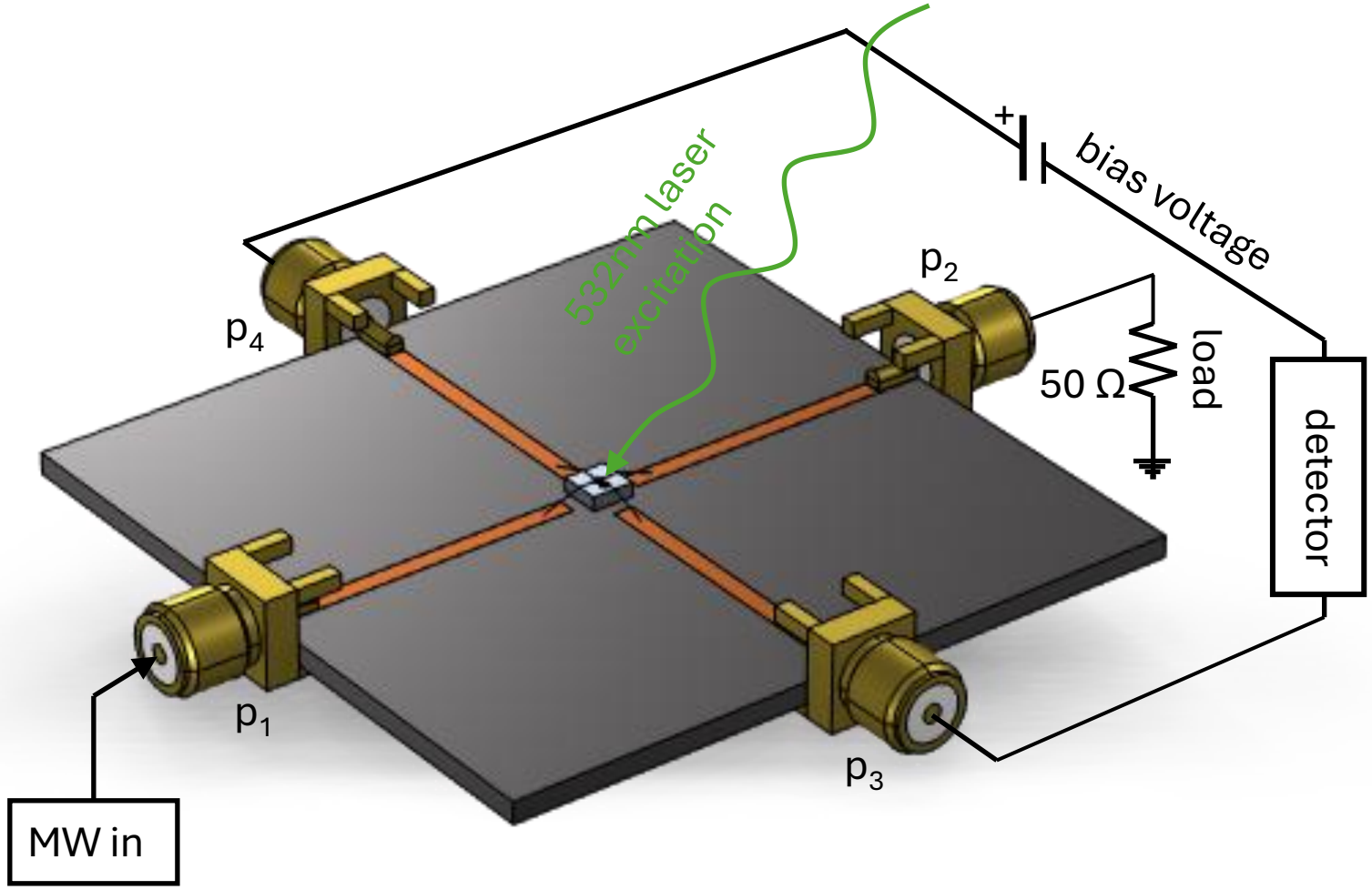
MOTIVATION

Investigate role of the crystalline environment

Investigate the diamond/electrode boundary

Goal:

Development od the unified tool for the prediction of photocurrent response of NV



Schema of chip connected for PDMR

Thin structure design

Ti/Au Ti/Al 20/100nm

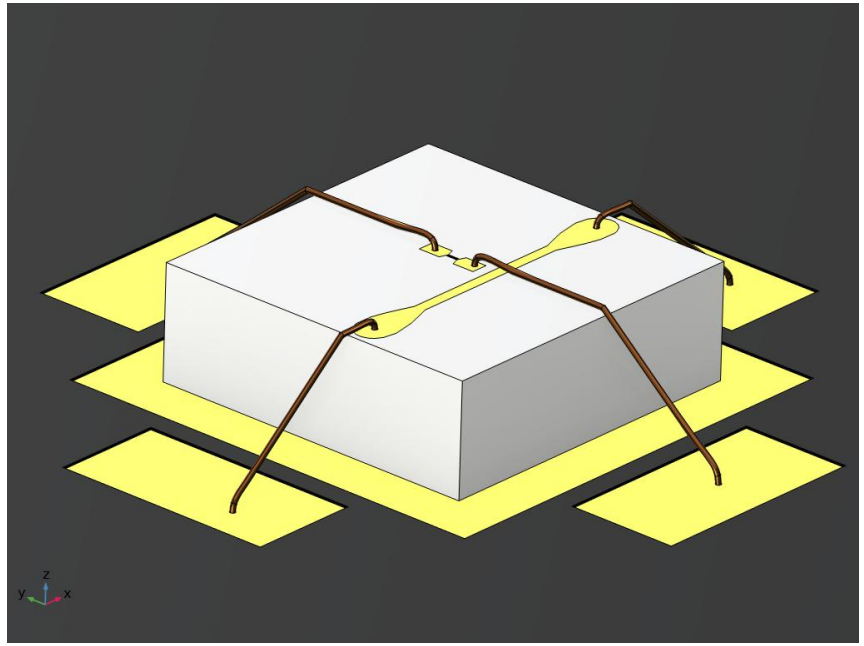
Negative UV photolithography

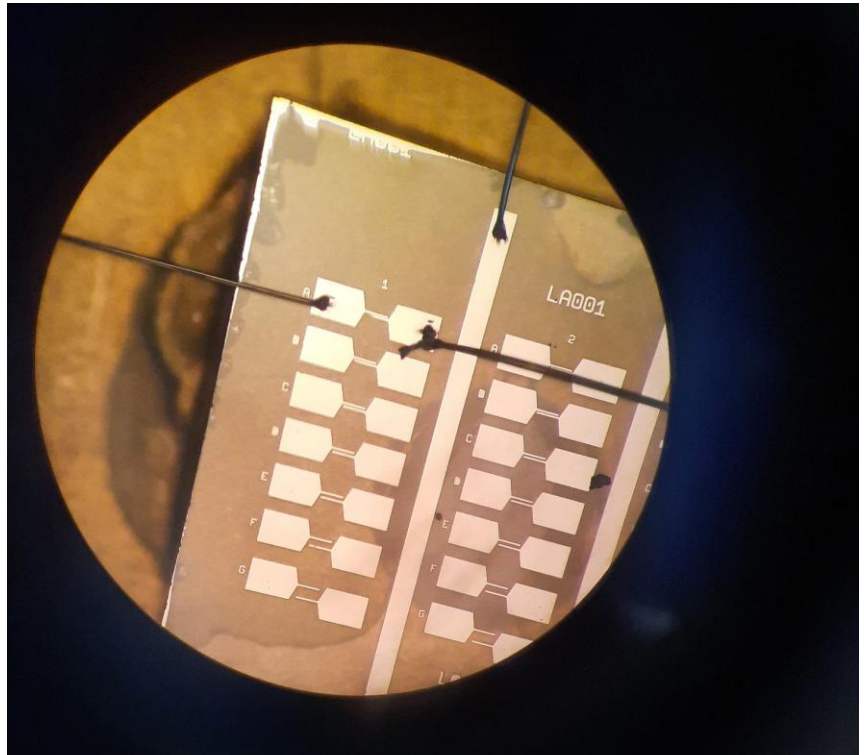
Line electrodes with variation of the gap (5-30um)

Applied voltage +- 3V/um
MW power 1mW- few W (freq 2-4GHz)

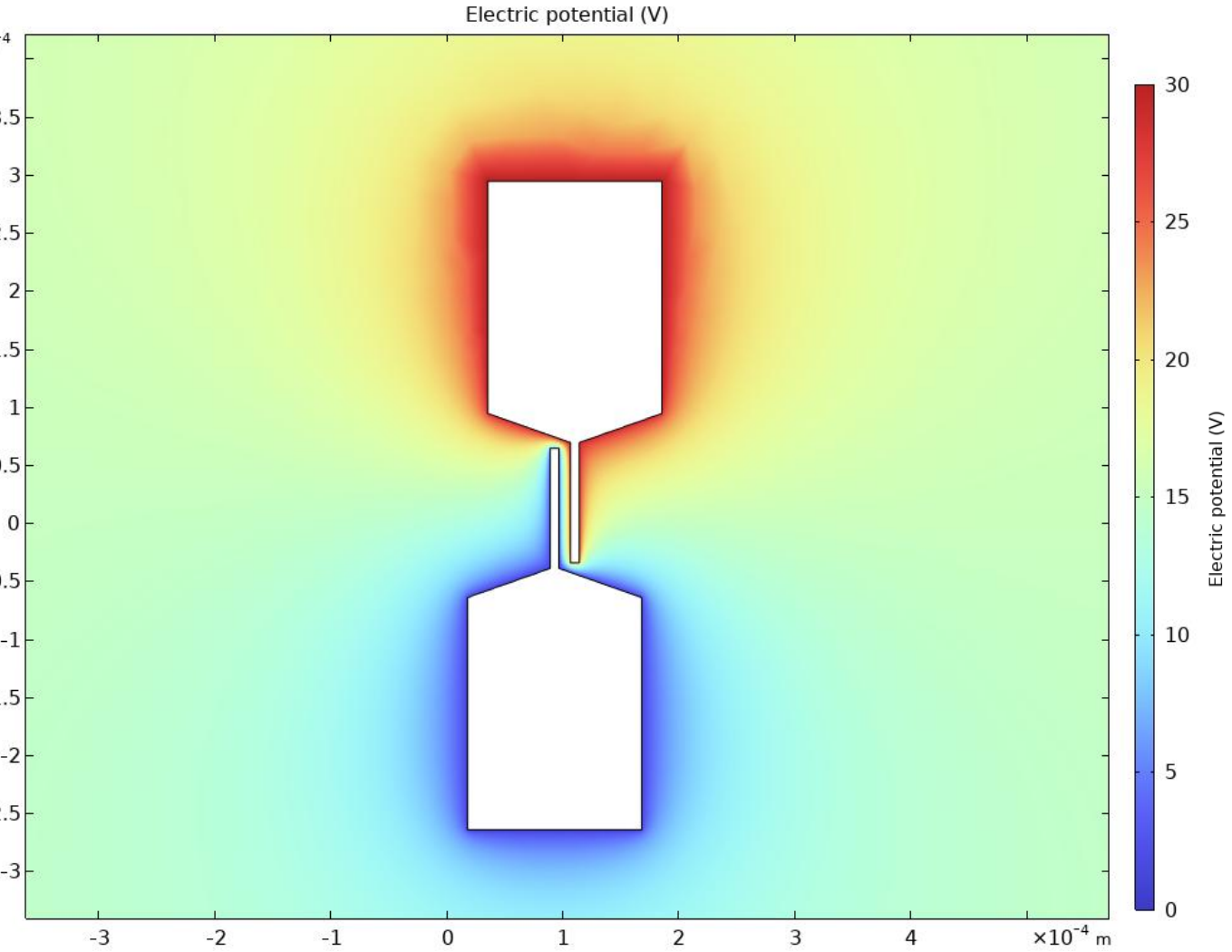
Detected currents (depend on doping) 100fA – 100pA

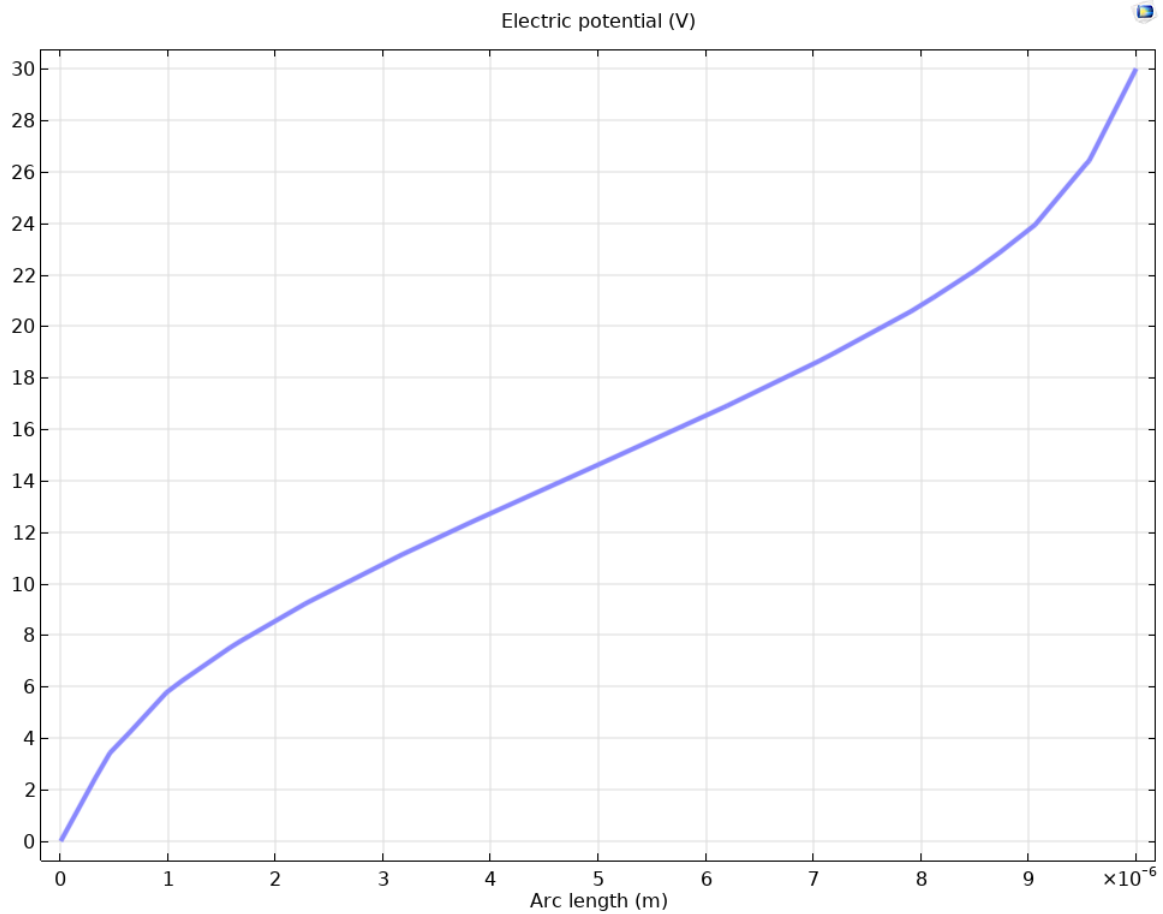
Simulation of DC electrical and MW field distribution



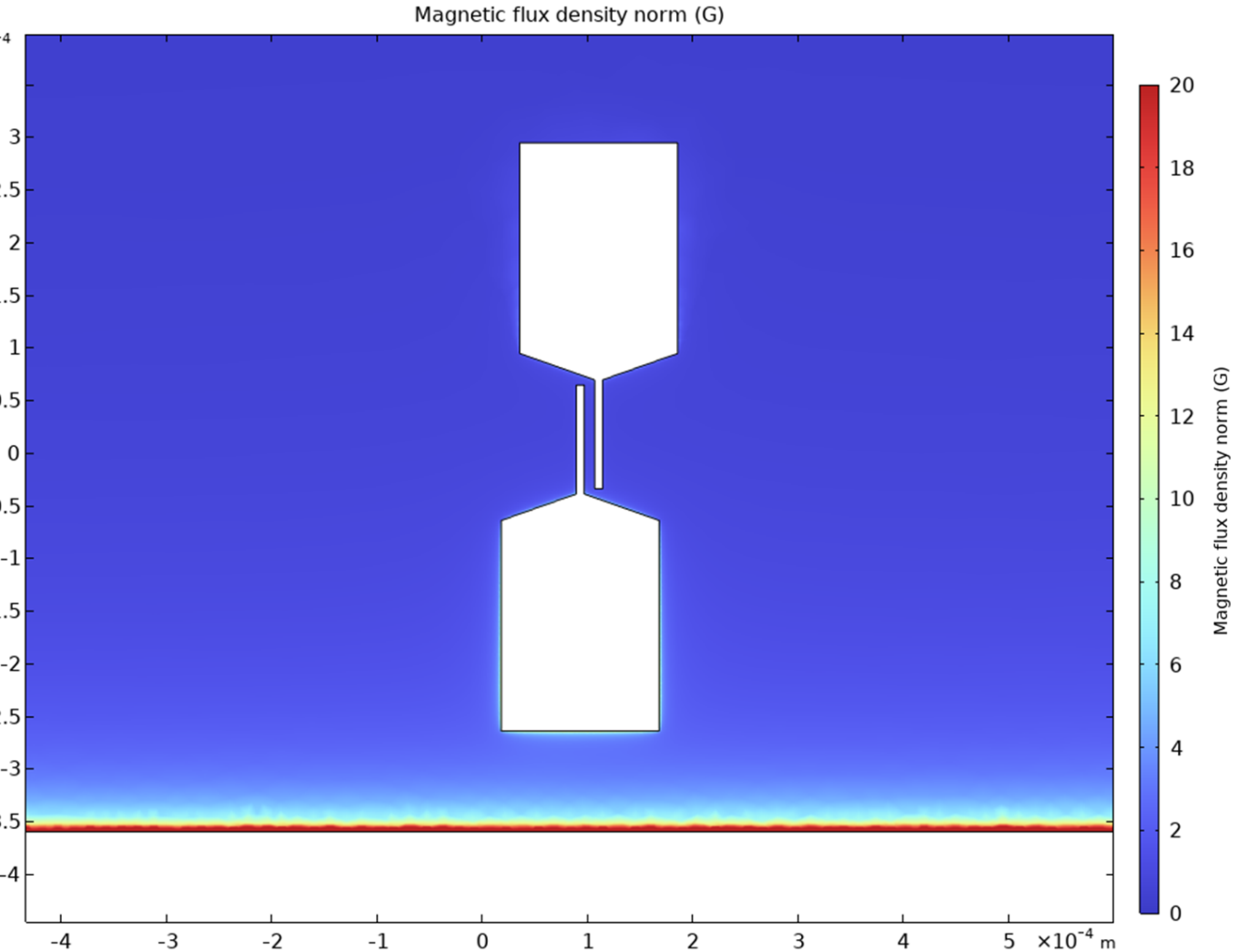


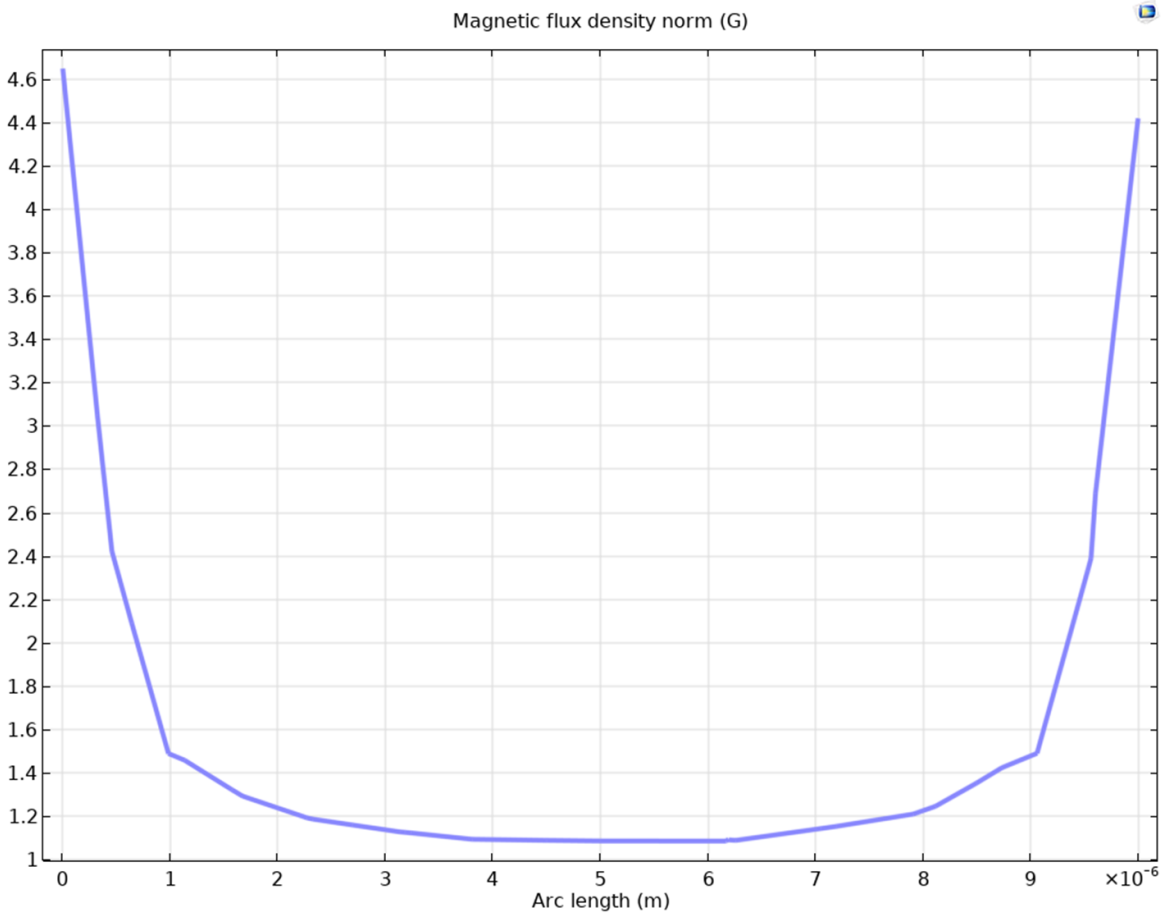
Bias DC field





MW field


Magnetic flux density norm (G)
Magnetic flux density norm (G)
20
18
16
14
12
10
8
6
4
2
0
-4
-3
-2
-1
0
1
2
3
4
5
×10⁻⁴ m


Magnetic flux density norm (G)
4.6
4.4
4.2
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0
1
2
3
4
5
6
7
8
9
×10⁻⁶
Arc length (m)

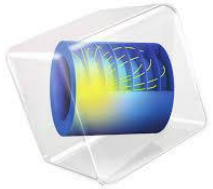
Multiphysics engineering

Simulation of the microwave excitation and electric field

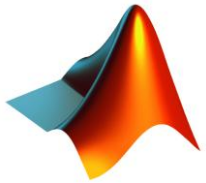
Simulation NV / charge carrier dynamic

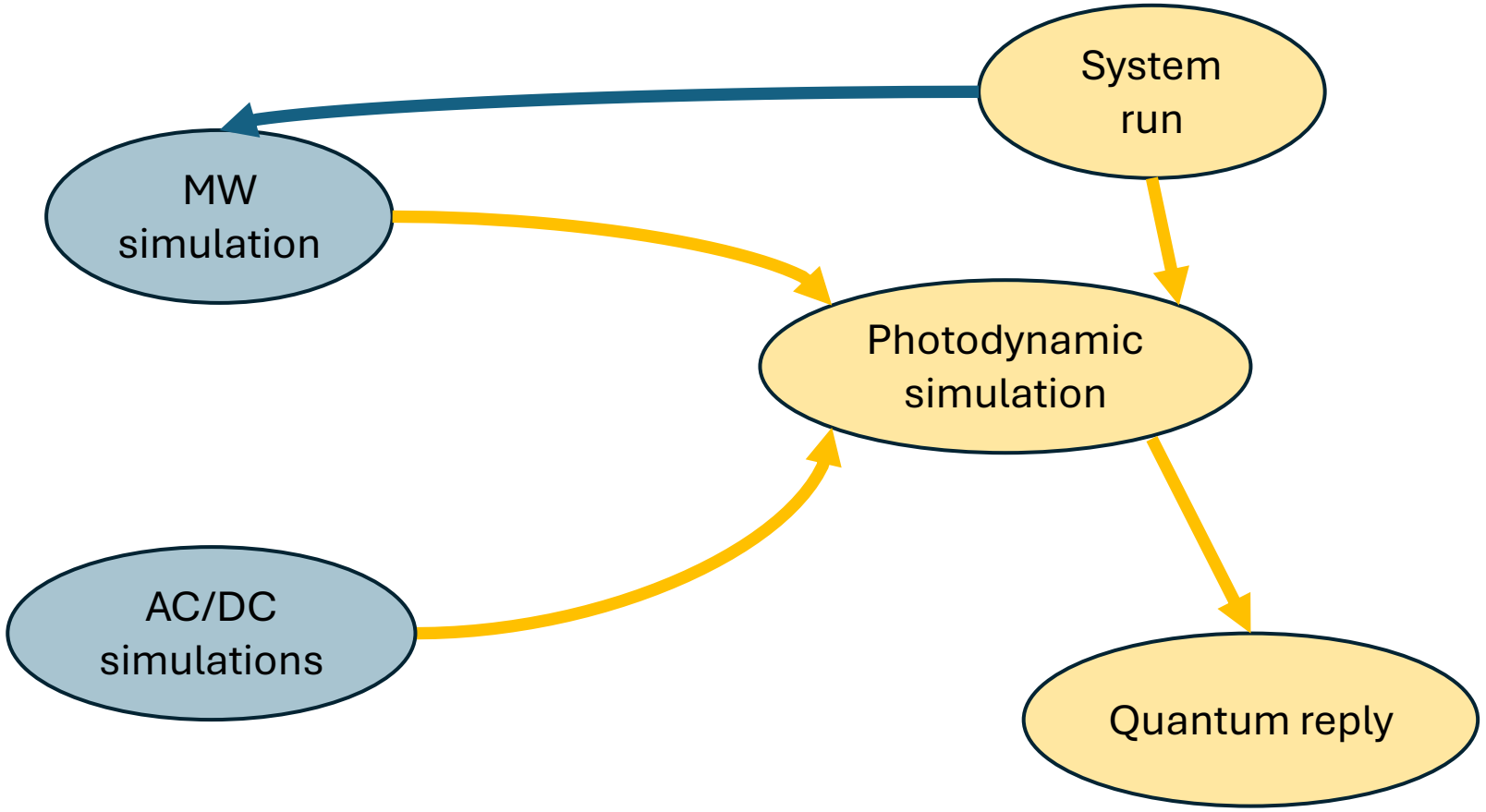
Calculation of the NV quantum response (contrast, defect related photocurrent…)

Chip designing and ‘macro’ modelling



Event triggering, Quantum modelling

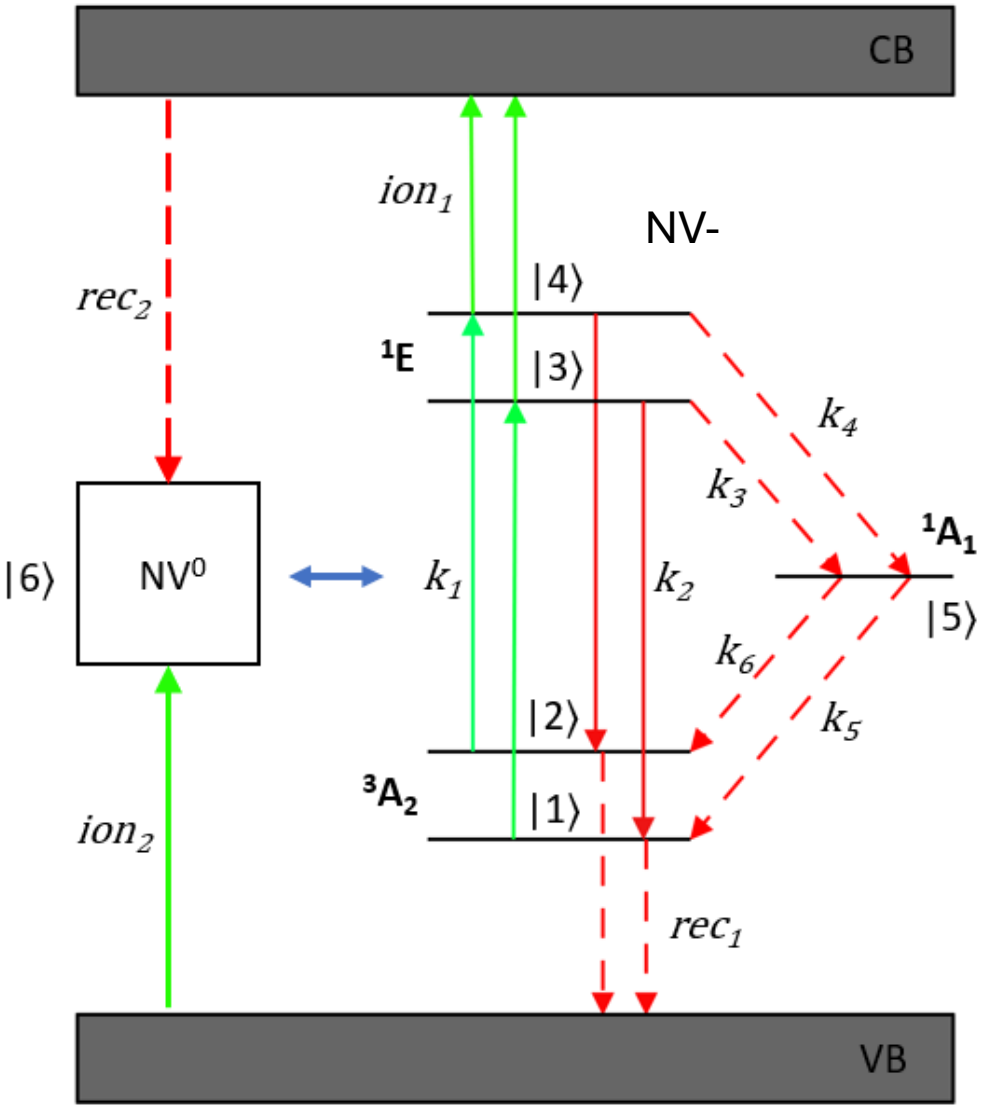




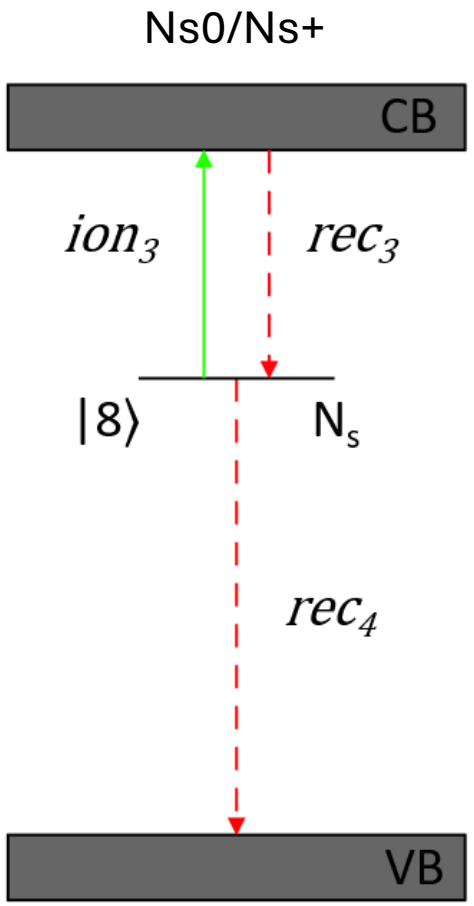
Quantum physics

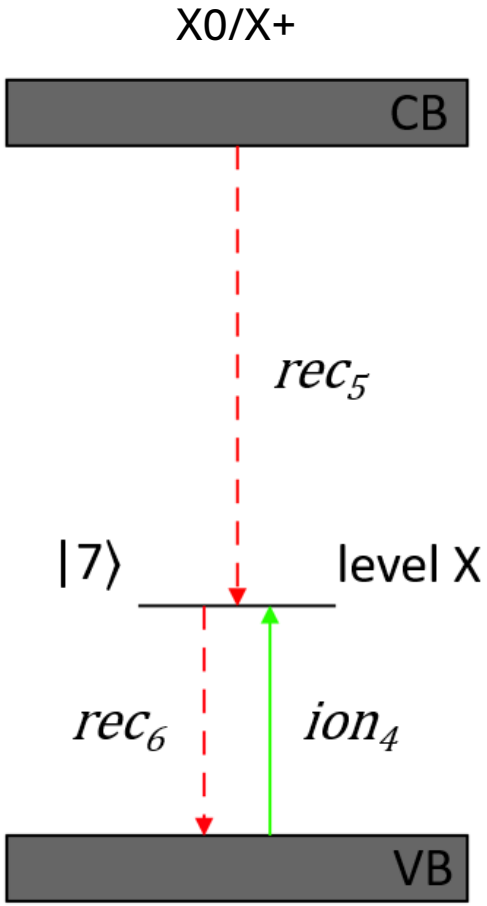
J. Soucek et. al. Phys. Rev. App. 2024

E. Bourgeois, J. Soucek et. al. Adv. Quant. Tech., 2022



NV0/NV-





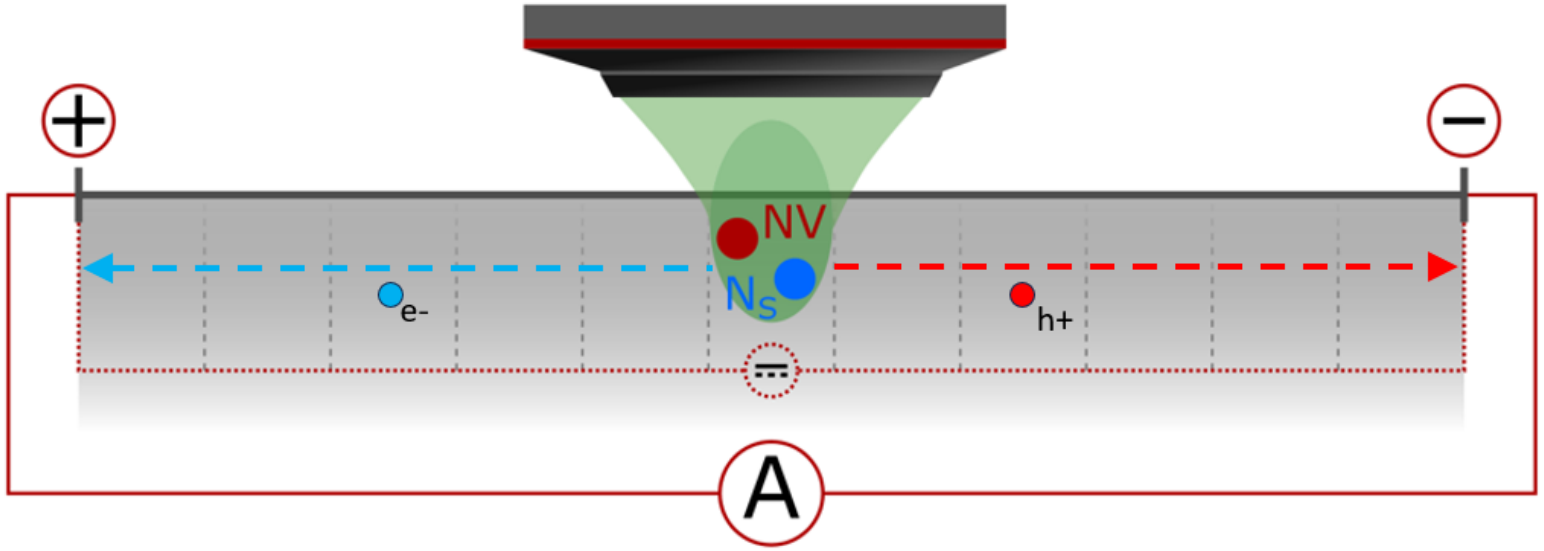
$$\frac{p_{|4\rangle}}{dt} = k_1 \cdot p_{|2\rangle} - (k_2 + ion_1 + k_4) \cdot p_{|4\rangle}$$

J. Soucek et. al. Phys. Rev. App. 2024
E. Bourgeois, J. Soucek et. al. Adv. Quant. Tech., 2022

1D channel approximation Ordinary Differential Equations -> Partial Differential Equations

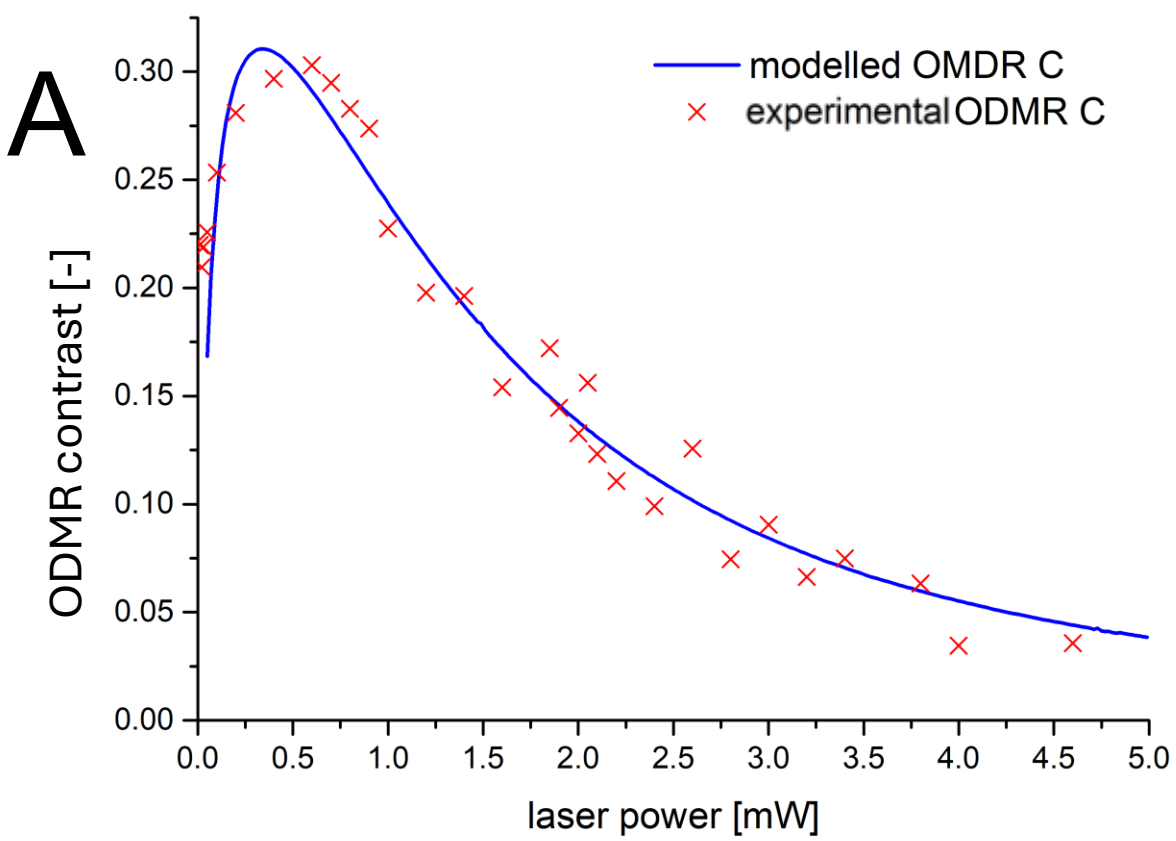
Drift/Diffusion of charge carriers (Boltzmann transport equations)

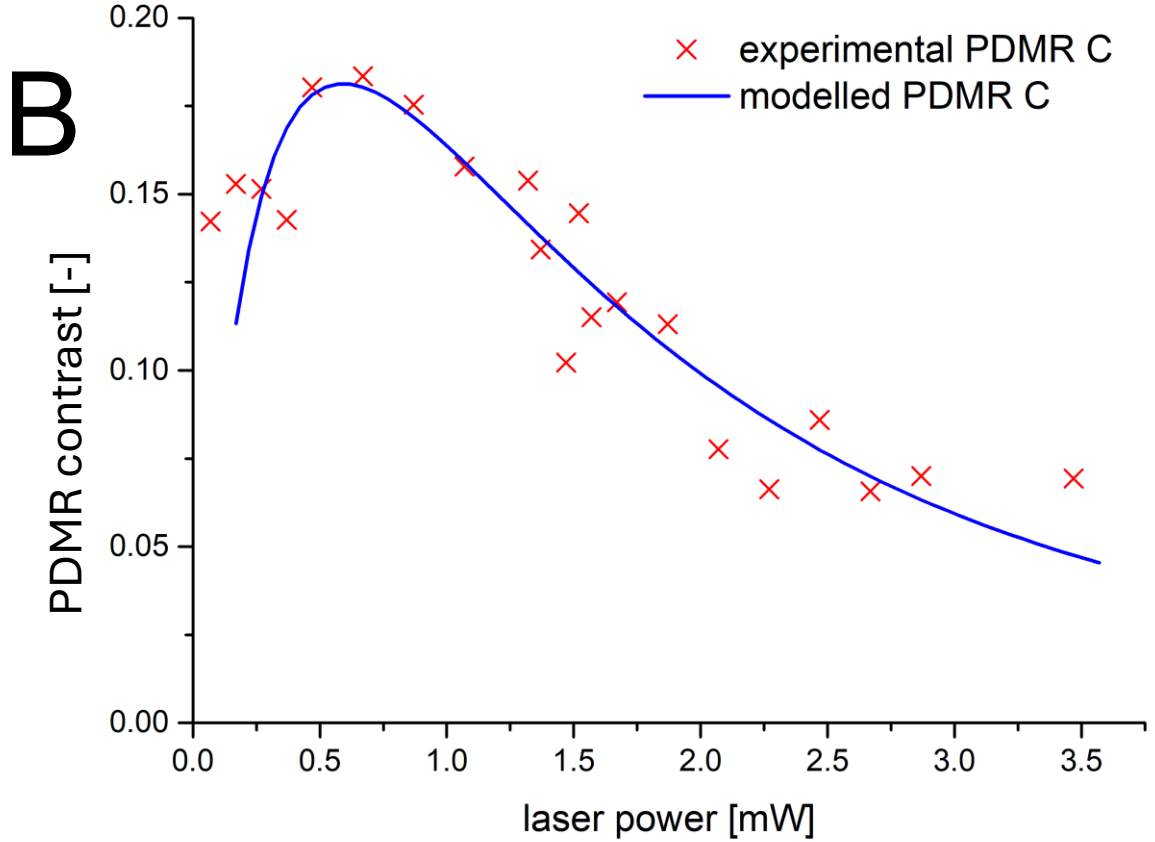
Trap/recombination implementation – additional photodynamic



J. Soucek et. al. Phys. Rev. App. 2024, in review

Model verification





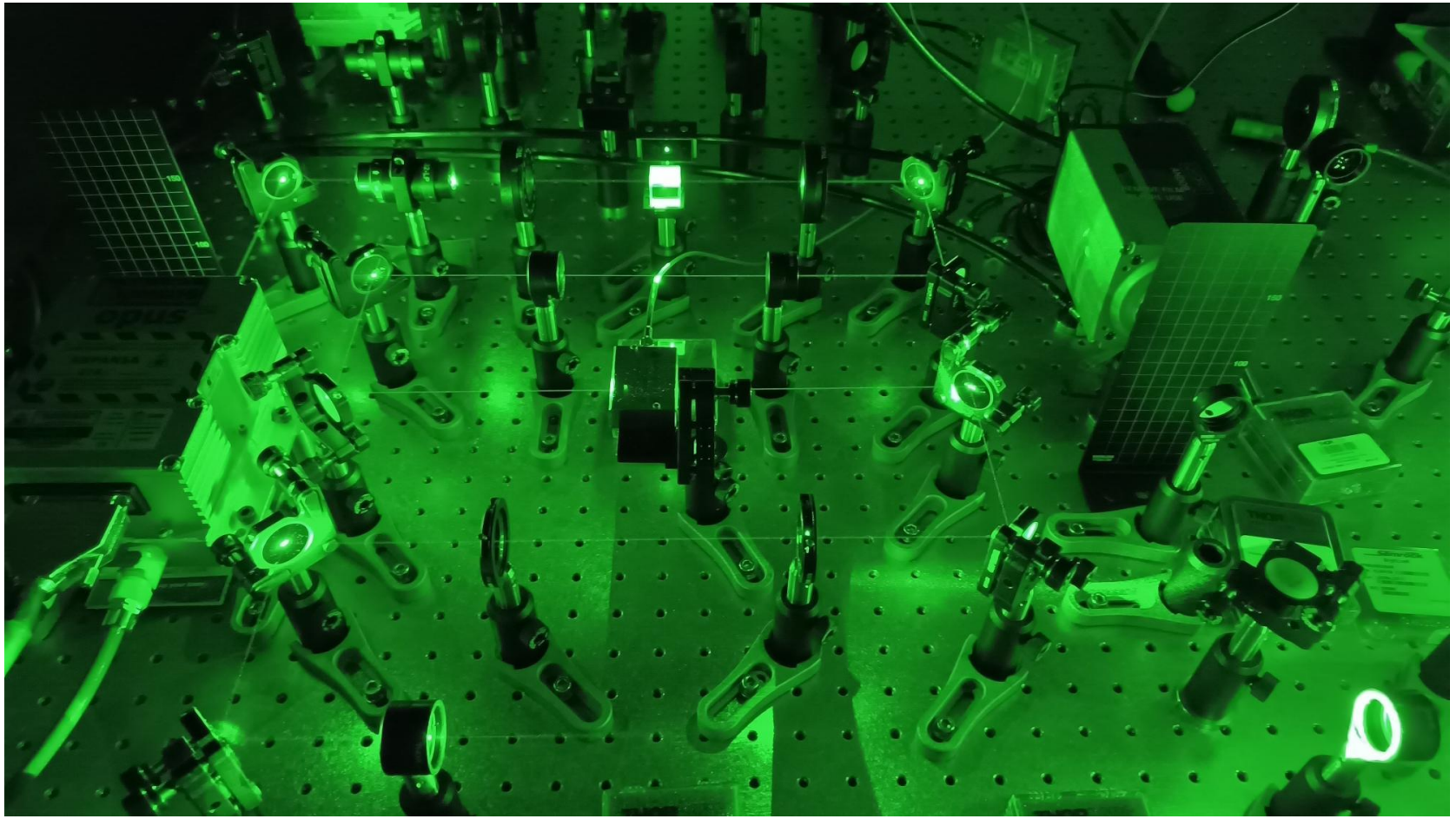
Modelling results for 1x NV, 10x Ns

Conclusion

Model that combines the ‘macro’ with ‘nano’ modelling

Verified by experiment

Allows us to design chip tailored for your material



Thanks for the attention