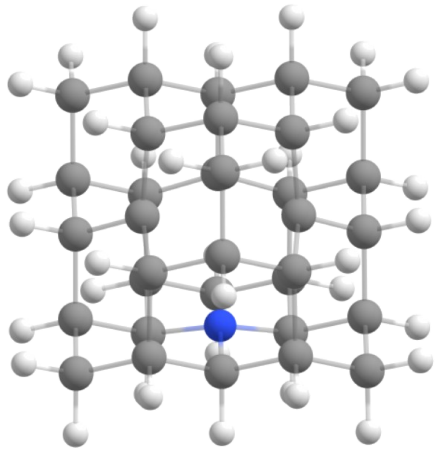
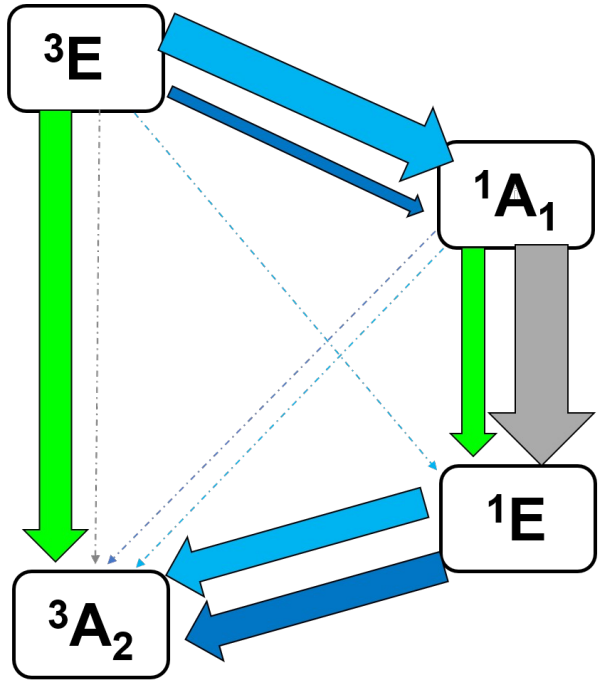
Quandidate

Empowering quantum chemistry to find novel point defect quantum bits

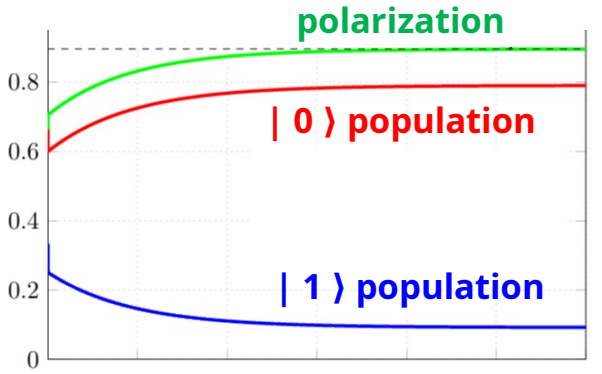


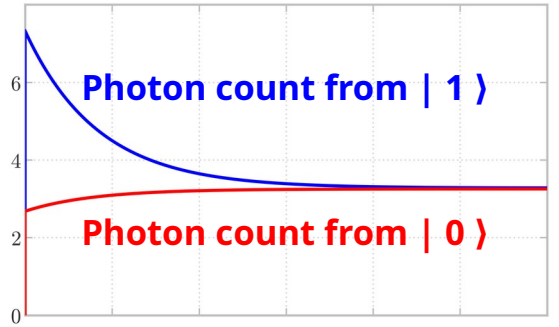
Defect **candidate**

Quandidate



Electronic states, **quan**titative rate model



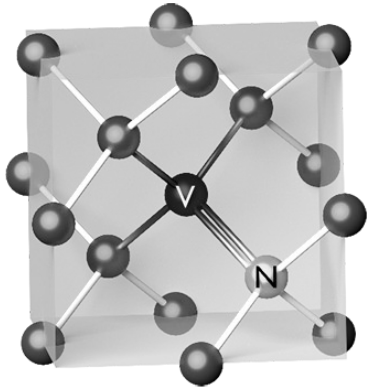


Simulation of **qu**bit initialization and readout

Qutility

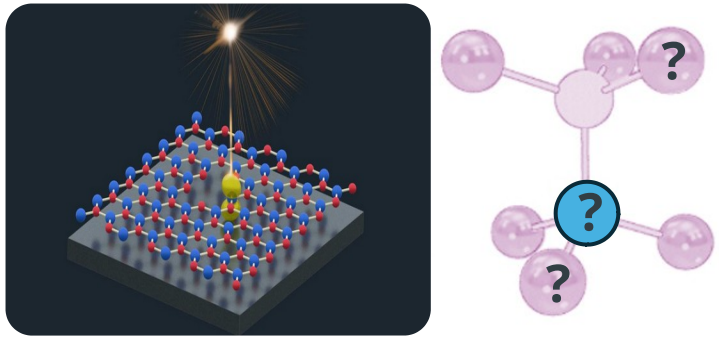
The quest to find NV^- alternatives

The present of defect qubits:
NV- in diamond



- Well-characterized qubit properties…
- … which became clear after decades of research
  Spectroscopy, pulsed spin, ODMR, single-photon correlation, electronic structure theory, etc.

The future of defect qubits:
(any defect) in (any crystal)

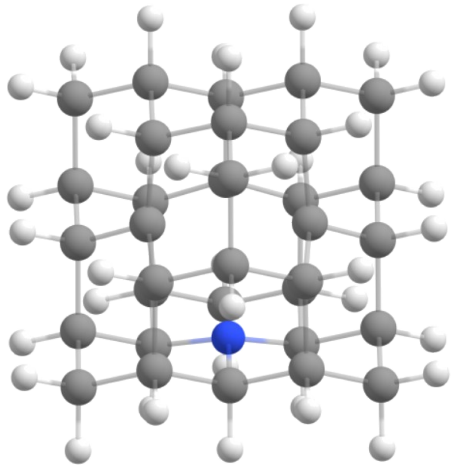


- The possibilities are endless!
- No time for long research on a single defect!

Qutility

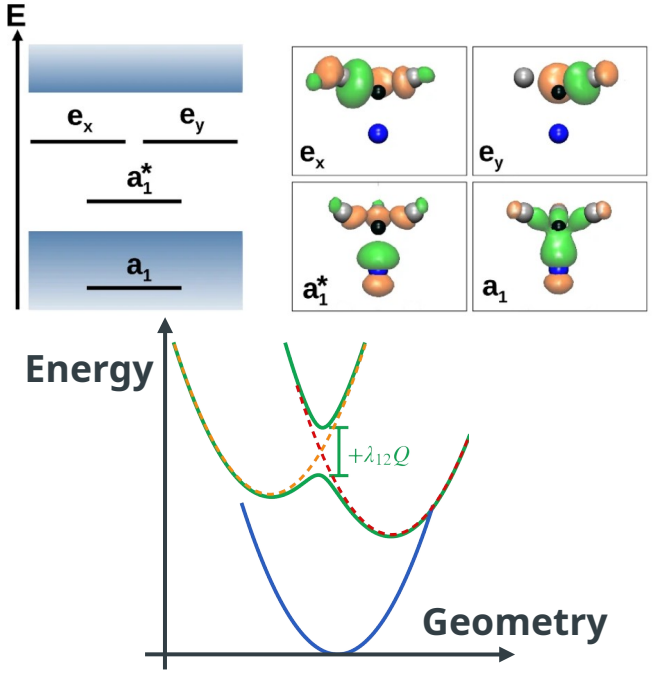
Quandidate:
a shortcut to full qubit characterization

INPUT:



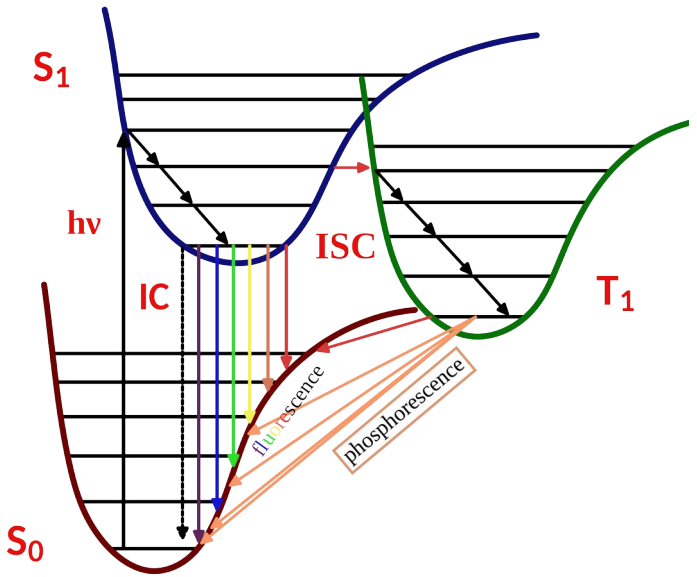
Defect model

PHASE 1



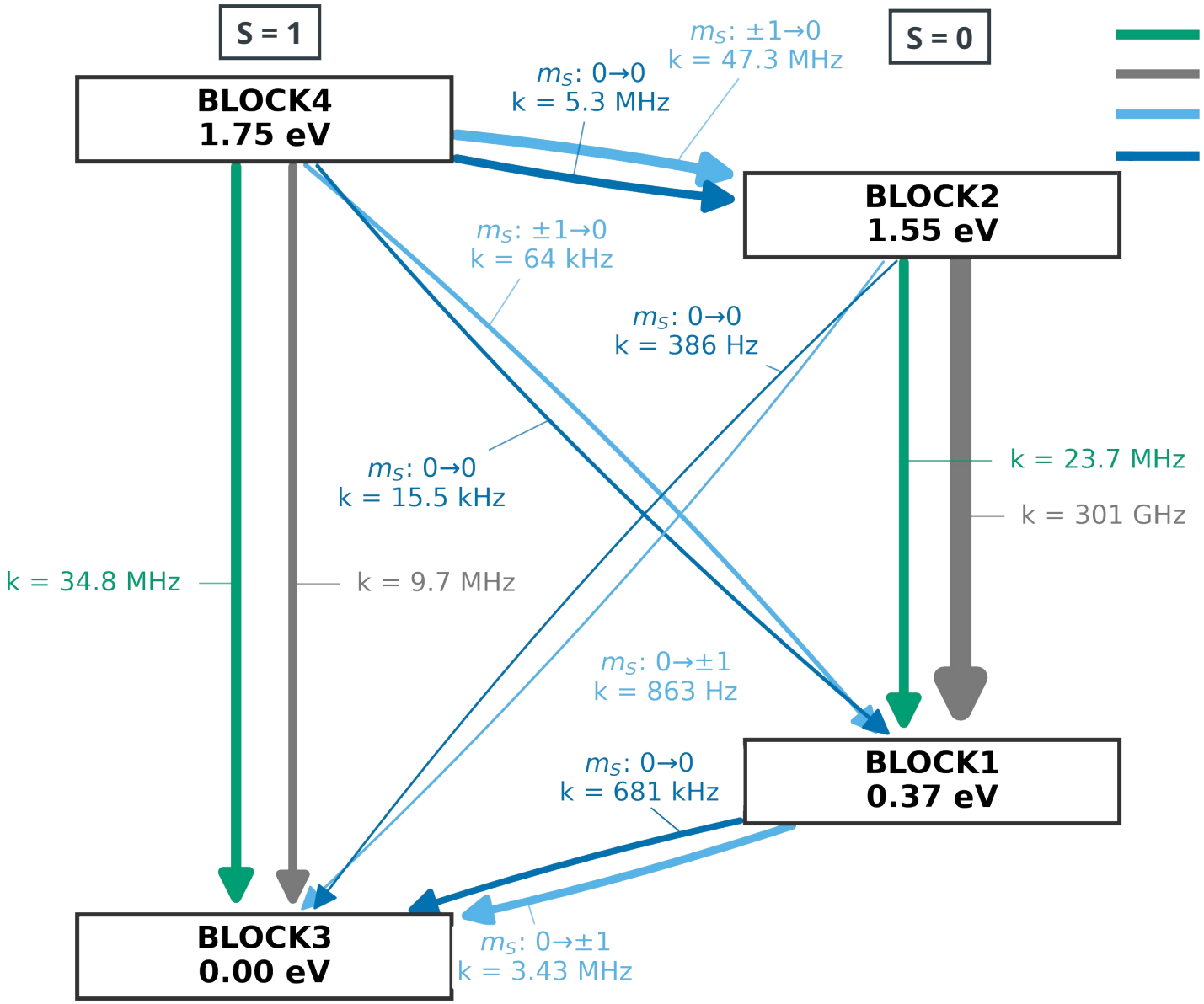
Automated high-level quantum chemistry

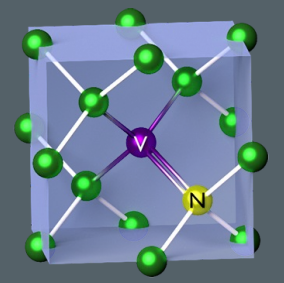
PHASE 2



Automated high-level excited-state dynamics

Qutility





- Actual Quandidate results for NV- in diamond (small model)
- Accessible within a few 100 CPU hours
- Remarkable agreement to experimental rates

Qutility