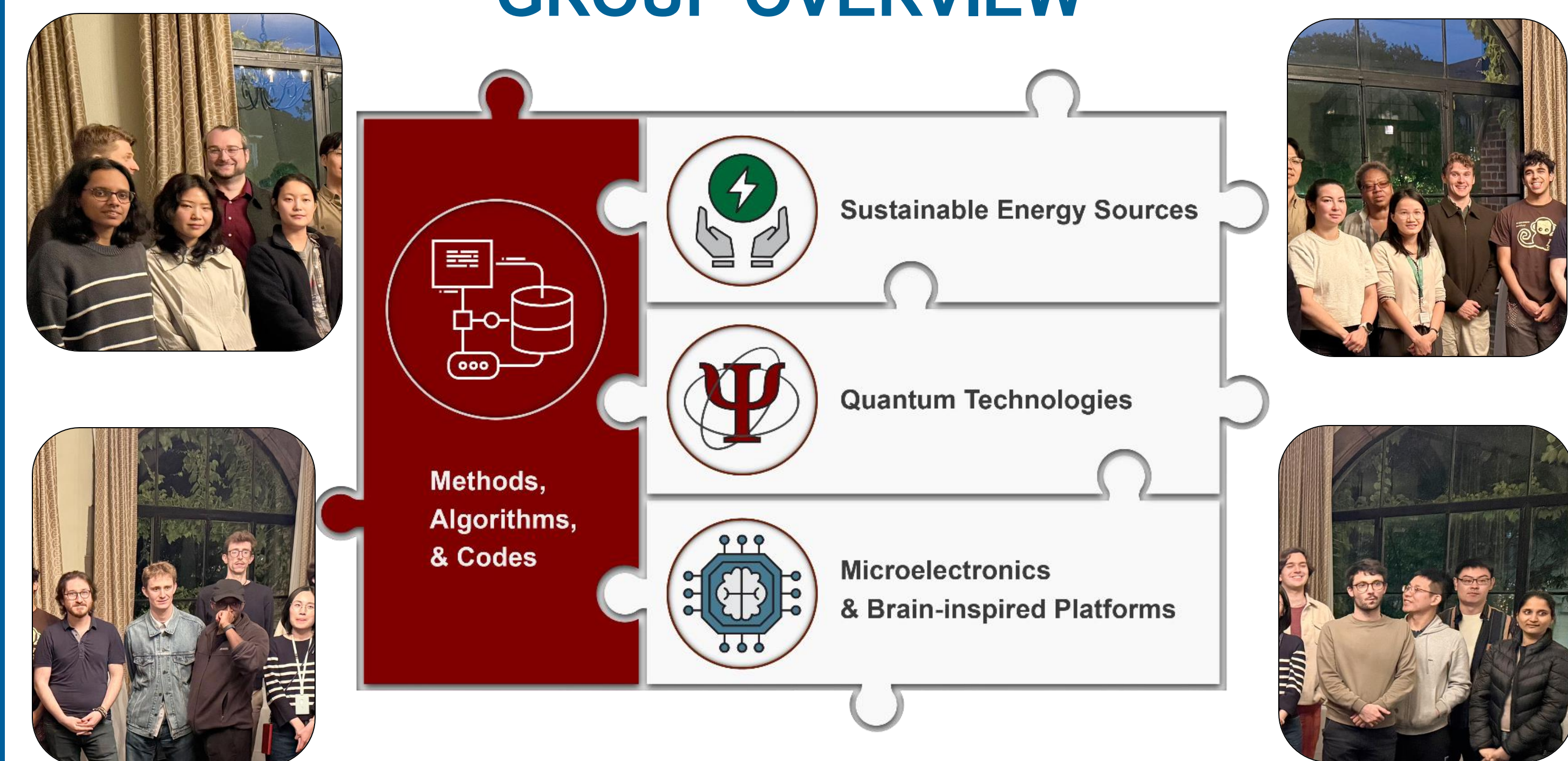


We develop theoretical and computational methods to predict and engineer the properties of materials and molecules

GROUP OVERVIEW



DEVELOPMENT OF METHODS AND CODES

We develop and use **methods based on quantum mechanics** and **open-source software** to understand and predict the properties of solids & molecules at the microscopic scale

Time-dependent density functional theory (TDDFT)
Jin, Yu, et al., J Chem Theory Comput. 2023; Zhan & Galli Chem. Theory Comput. 2026

Many-body perturbation theory (MBPT)
Govoni & Galli, J Chem Theory Comput 2015, 2018; Yu & Govoni, J Chem Theory Comput 2022; Yu et al., J Chem Theory Comput 2024

Quantum defect embedding theory (QDET)
Sheng et al., J Chem Theory Comput 2022; Vorwerk et al., Nat Comput Sci 2022; Chen, Yu, et al., J Chem Theory Comput 2025

Cluster-correlation expansion (CCE)
Onizhuk & Galli, Rev Mod Phys 2025; Nagura, Jonah et al. Phys. Rev. Mater.

Hybrid density functionals
Zhan et al., J Chem Theory Comput 2023, Phys Rev Mater 2025

Stochastic methods for electron-phonon interaction
Kundu & Galli, J Chem Theory Comput 2023, J Phys Chem Lett 2024

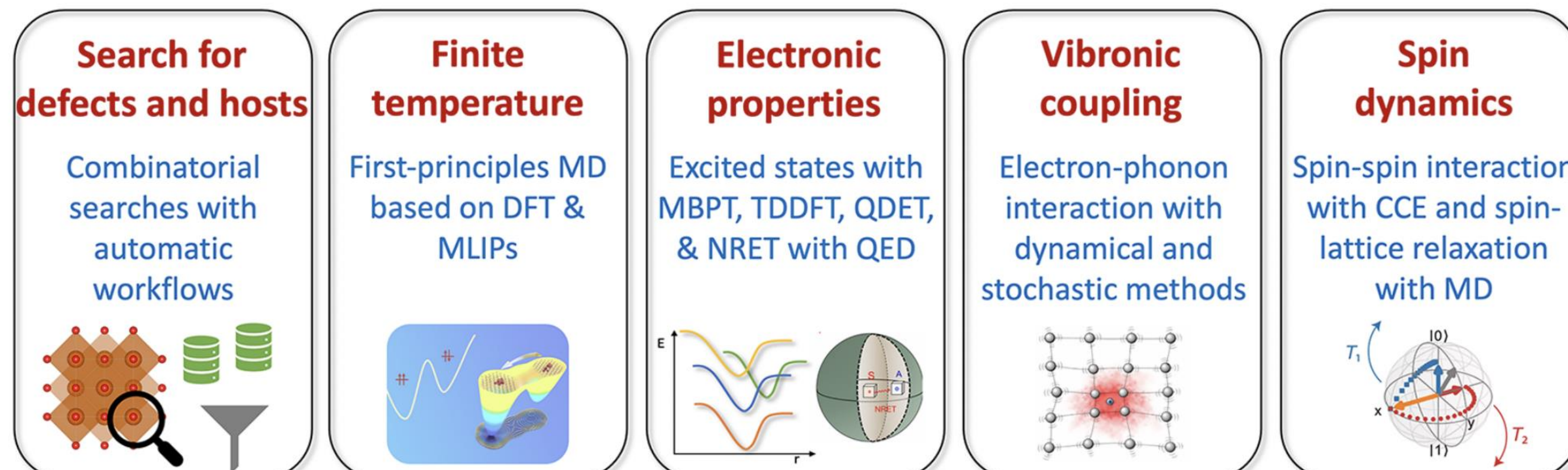
First principles molecular dynamics and machine learned interatomic potentials.
Drigo et al., 2026 (arXiv: 2605.04294); Bousquet et al. 2026 (arXiv:2607.08617)

<WEST!>

pycce

Qbox
First-Principles Molecular Dynamics

INTEGRATED CAPABILITIES AT WORK



Scaling of algorithms & Simulations of realistic systems in collaboration with experiments

For all properties, highly scalable, parallel codes, on CPU & GPU

Excited states (Fermionic Hamiltonians) on quantum computers
VQE & Shadow tomography-based algorithms + noise mitigation

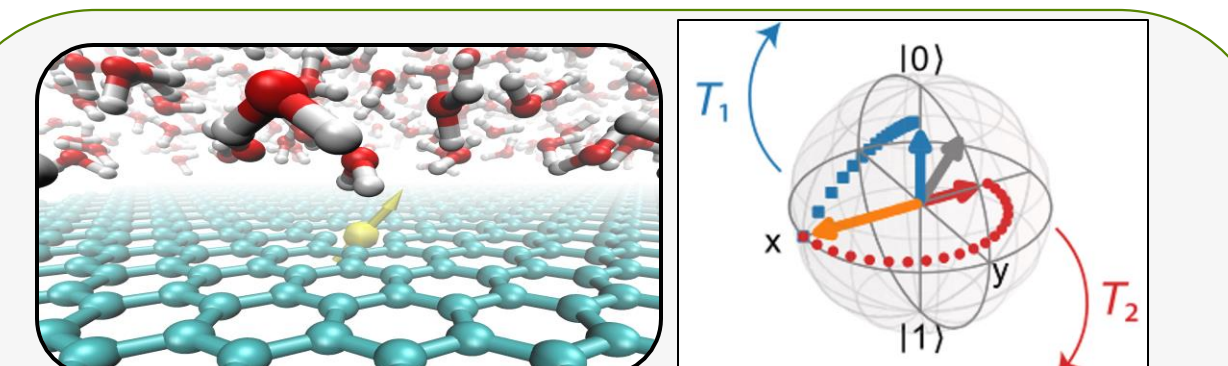
Galli et al. J. Chem. Theory Comput. (2026)

MATERIALS FOR QUANTUM TECHNOLOGIES

What are the **properties of defects** that can be used to store quantum information?

How **stable** are defect-based qubits? Can we **engineer** their environment?

How do they **interact with light**? How can we control them?

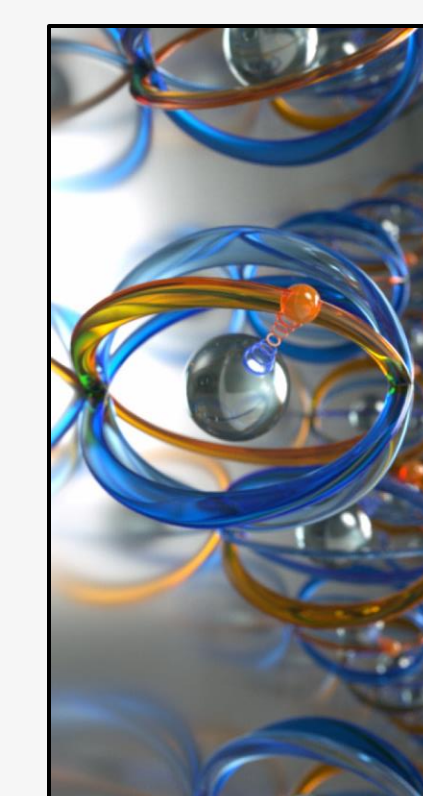


Can we use defects in quantum materials as **quantum sensors**?
Can we engineer **entangled quantum defects**?
Can we predict materials for **quantum communications**?

How can we model the dynamics of spin in complex materials?

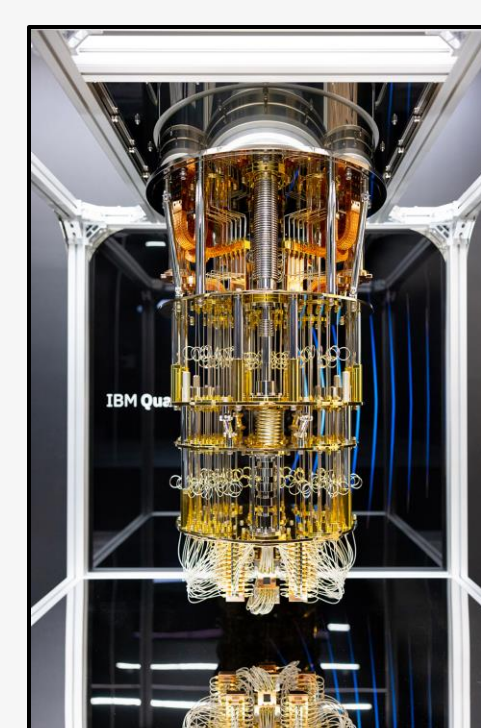
How long do the state of spin defects remain **coherent**?

What processes control coherence?



Can we use quantum computers to model quantum materials?

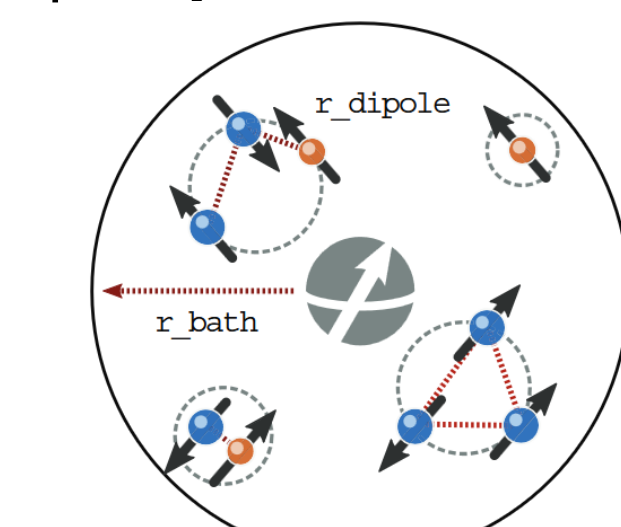
What are the **algorithms** required for efficient quantum simulations?



UNDERSTANDING COHERENT STATES

We are interested in the **properties of spin defects** both inside the bulks of materials and near surfaces and interfaces

Interacting spins can be modelled with a coupled cluster approach. We developed a community code (**PyCCE**) to simulate spin dynamics.

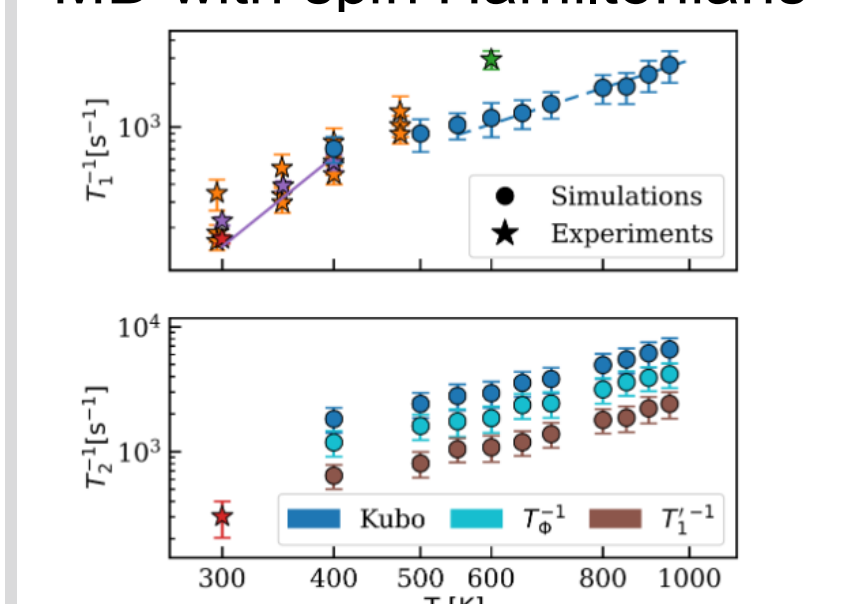


CITE REV MOD PHYS

Ongoing Investigations

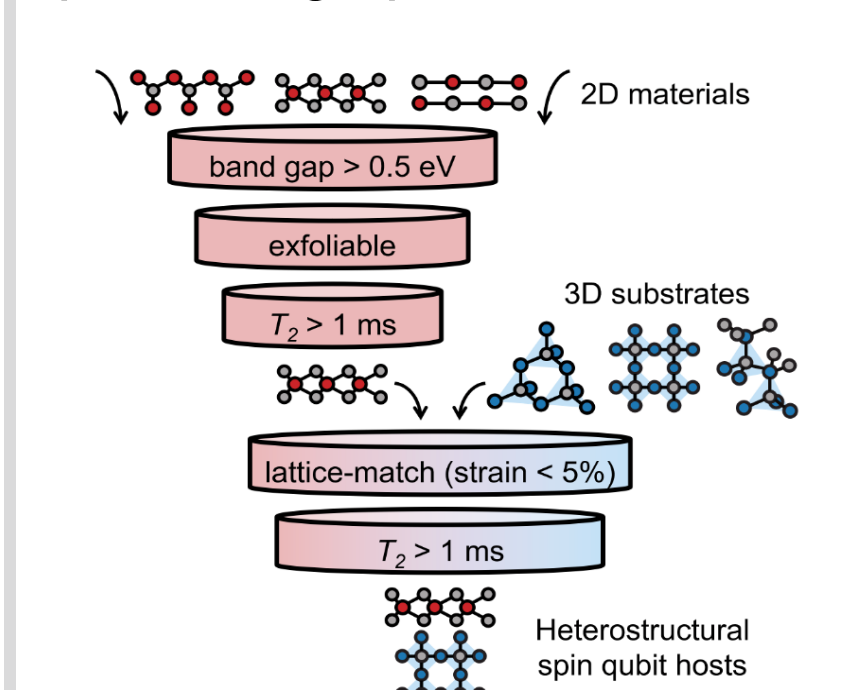
- Modeling **entangled spin defects**
- Modeling **molecular qubits**
- Modeling **quantum sensors in proximity of aqueous interfaces**
- Improving the efficiency of spin coherence calculations, using **NN and MLIPs**

We developed a framework to investigate **coherence times as a function of temperature** by coupling MD with spin Hamiltonians

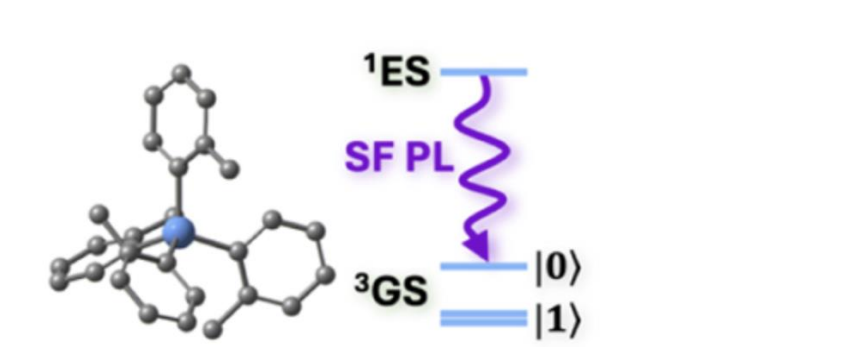
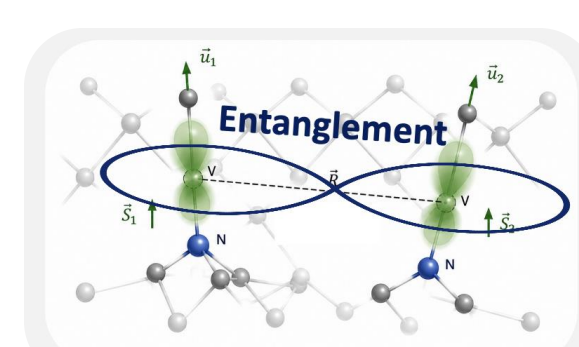


Drigo et al., 2026 (arXiv: 2605.04294)

We performed **materials screening** to determine promising spin defect hosts.

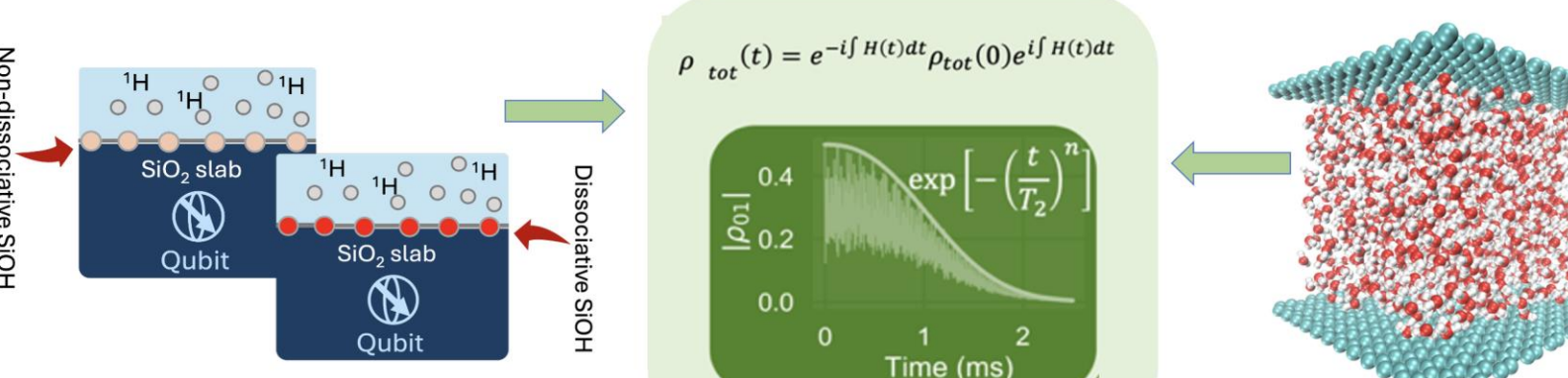


Toriya et al., npj 2D Materials and Applications 2025



D. Sorbelli and G. Galli, JACS Au 2026

Probing hydrophilic and hydrophobic interfaces



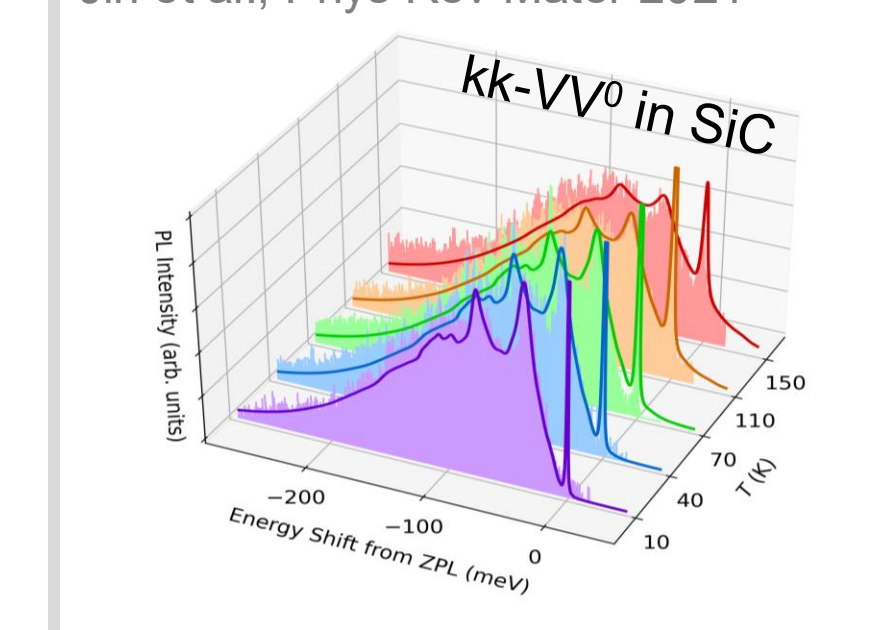
A. Castillo and G. Galli, JPC 2025

LIGHT-MATTER INTERACTION

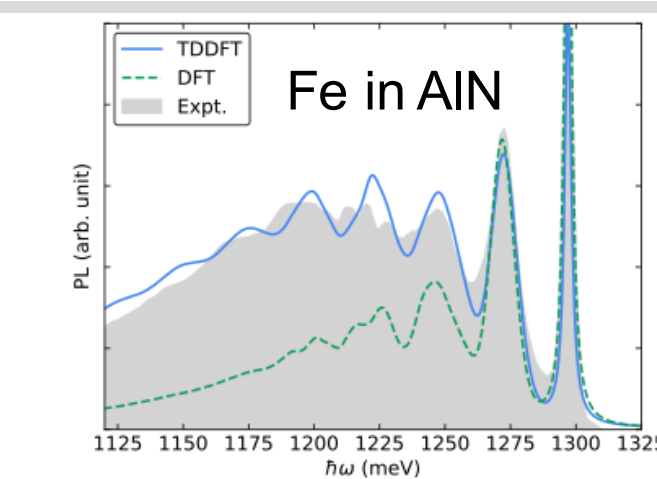
We developed methods and software to computationally characterize the complete **optical cycle** of spin qubits and **interpret and guide experiments**

Photoluminescence (PL) spectra as a function of temperature from **generating function approach**

Jin et al., Phys Rev Mater 2021

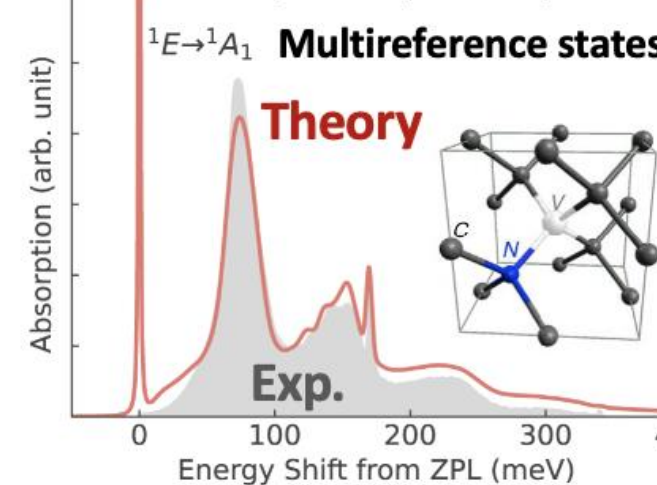


PL spectra of transition metal impurities in ionic crystals from spin-flip hybrid TDDFT w/ optimized excited-state geometries
Otis et al., J Phys Chem Lett 2025

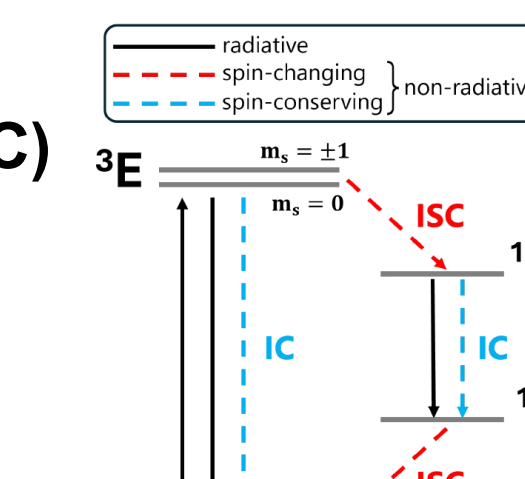


Absorption spectra between correlated states from **spin-flip hybrid TDDFT with optimized excited-state geometries**

Jin, Govoni & Galli, npj Comput Mater 2022

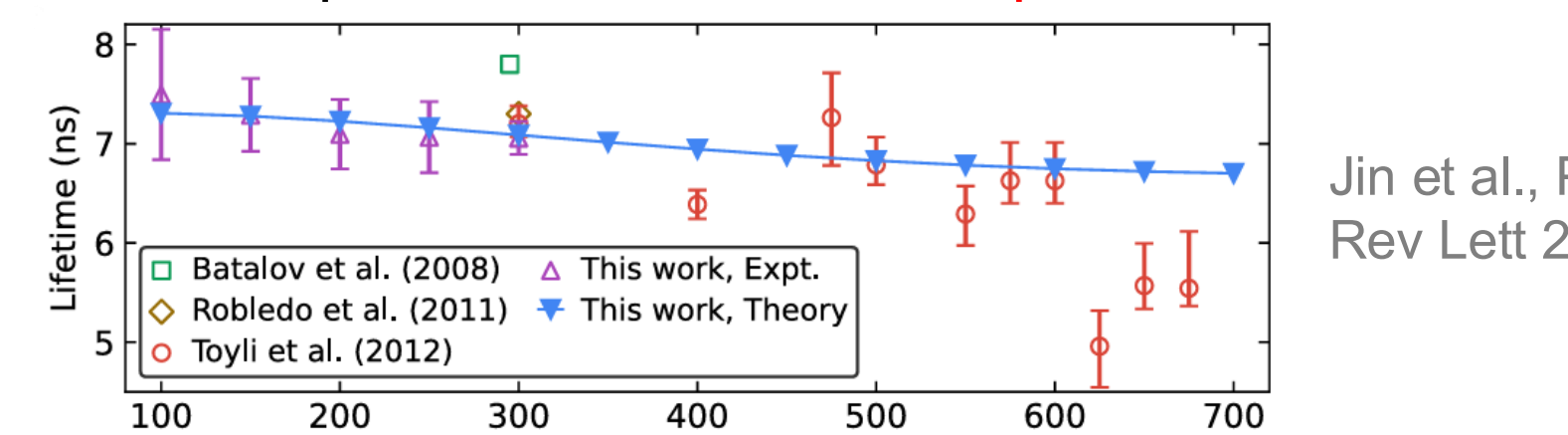


Inter-system crossing (ISC) rates and internal conversion (IC)



B. Huang, Y. Jin, GG et al. PRL 2026
S. Villani, Y. Jin and GG PRL 2026

- Excited-state geometries with **spin-flip hybrid TDDFT**
- Spin-orbit coupling matrix elements with multireference states from **QDET**
- Overlap functions with **ab initio phonons**

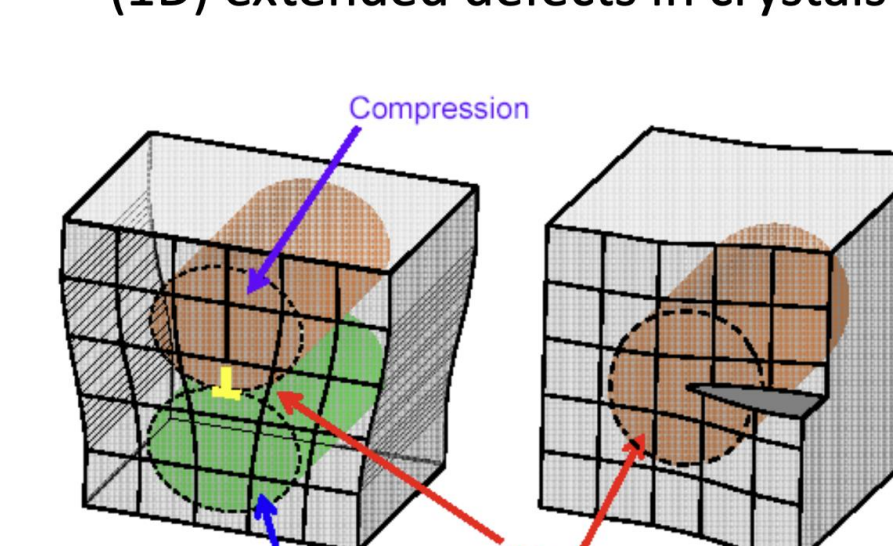


Jin et al., Phys Rev Lett 2025

QUANTUM DEFECTS IN COMPLEX SYSTEMS

Dislocations to design quantum interconnects

Dislocations are one-dimensional (1D) extended defects in crystals

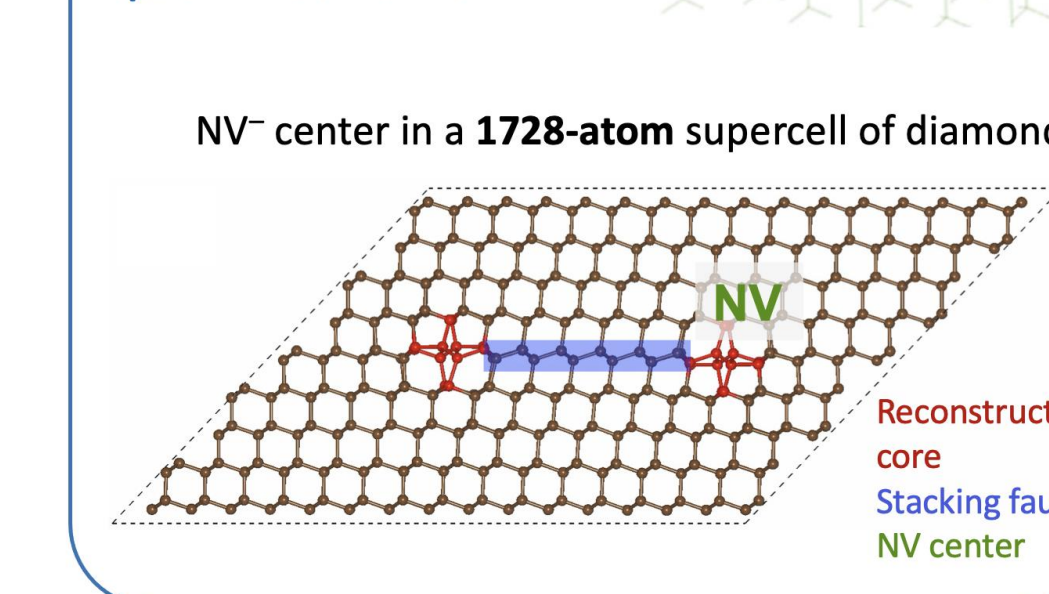


• Strain field along 1D edge and screw dislocations

• Core located at the center of the dislocation, where extreme distortions & reconstructions of the lattice geometry occur

C. Zhang et al., npj Comp. Mat. 2026

Use dislocations to engineer & entangle a qubit array for scalable solid-state qubit networks

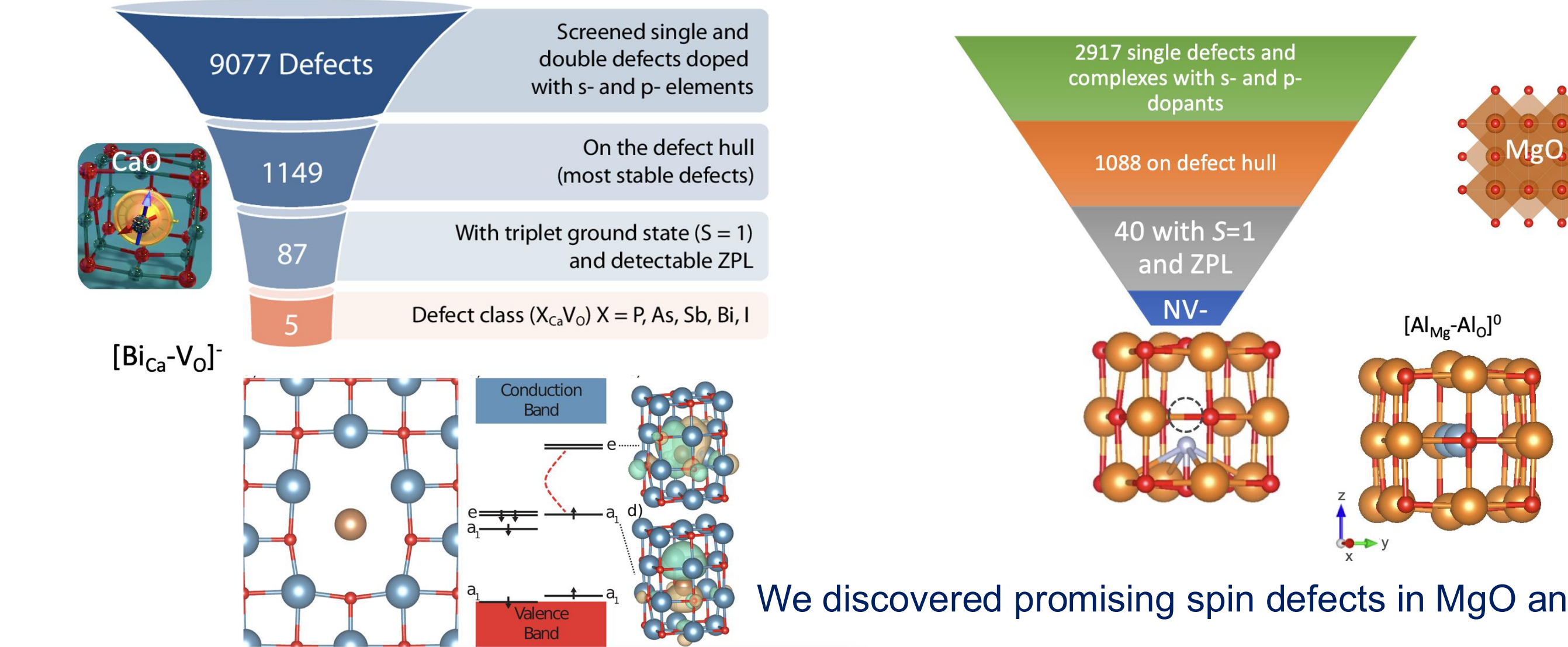


We identified several stable NV-centers located at dislocations

We predicted that an optical cycle for the initialization and readout of quantum states is feasible for NV-centers @ dislocations

High-throughput searches of defects in oxides

J. Davidsson, M. Onizhuk, C. Vorwerk, & GG Nat Commun 2024; V. Samjlit, J. Davidsson, Y. Jin & GG, npj Comp. Mat. 2025
S. Kanai et al. PNAS 2022



We discovered promising spin defects in MgO and CaO