HUN-REN
Hungarian Research Network

Wigner
All colors of Physics

BME PHYSICS
BMEatomfizika

HPC @hu
Kompetencia Központ

Spin-orbit-phonon relaxation in diamond qubits

WE WANT YOU

Ádám Gali's group

Komondor HPC
hungarian suprcomputer

M.Sc.

Point Defect modeling in semiconductors

Ph.D

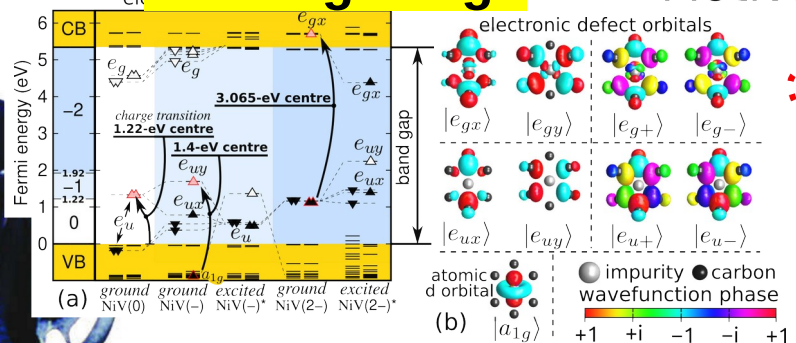
B.Sc.

ab-initio simulations at atomistic level by means of density functional theory

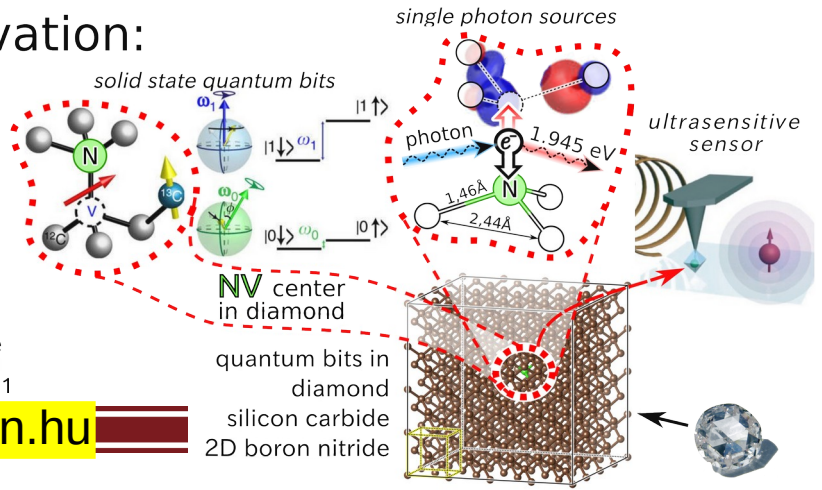
TDK

-electronic structure
-vibronic structure
-Jahn-Teller effect
-spin-orbit coupling
-photoluminsecence
-electron paramagnetic resonance

Thiering Gergő



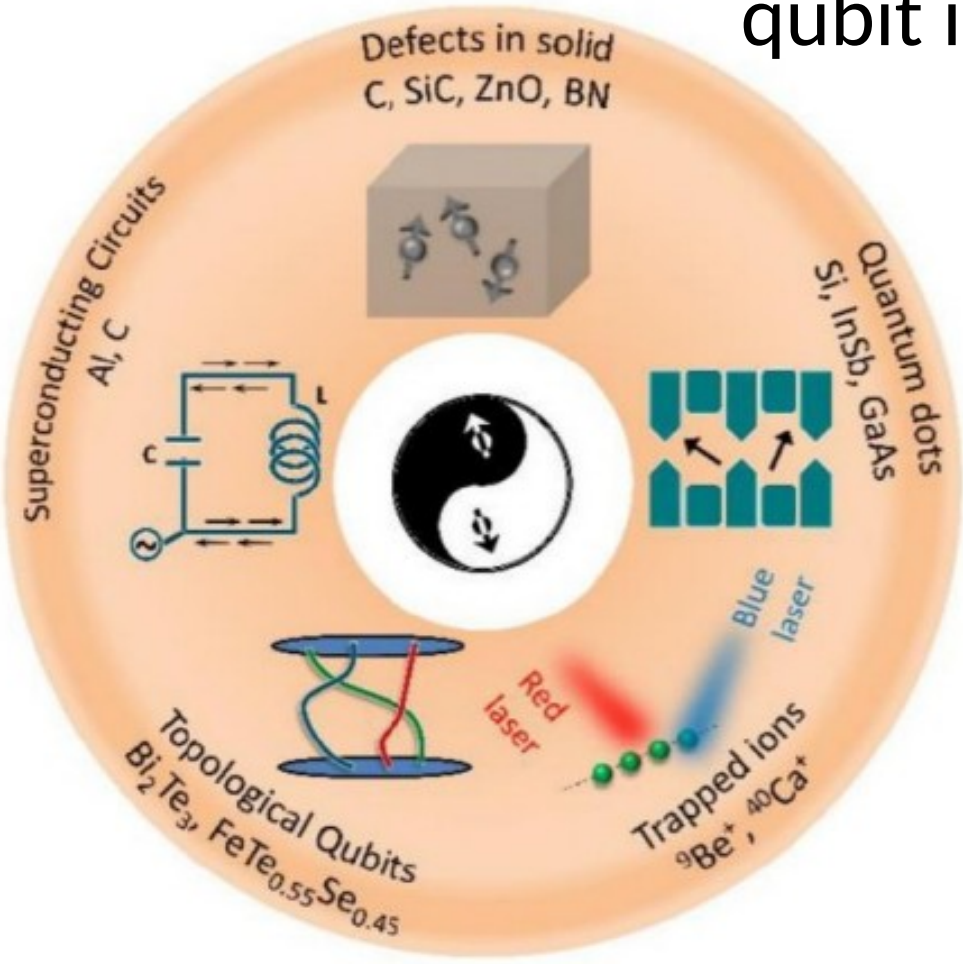
The Motivation:



thiering.gergo@wigner.hun-ren.hu
(gali.adam@wigner.hun-ren.hu)

Defects in semiconductors

qubit implementations

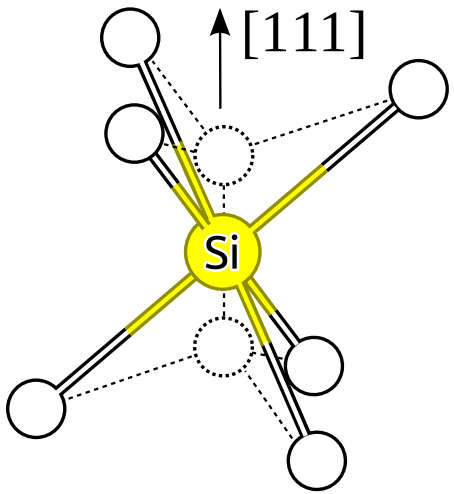


Defects in semiconductors

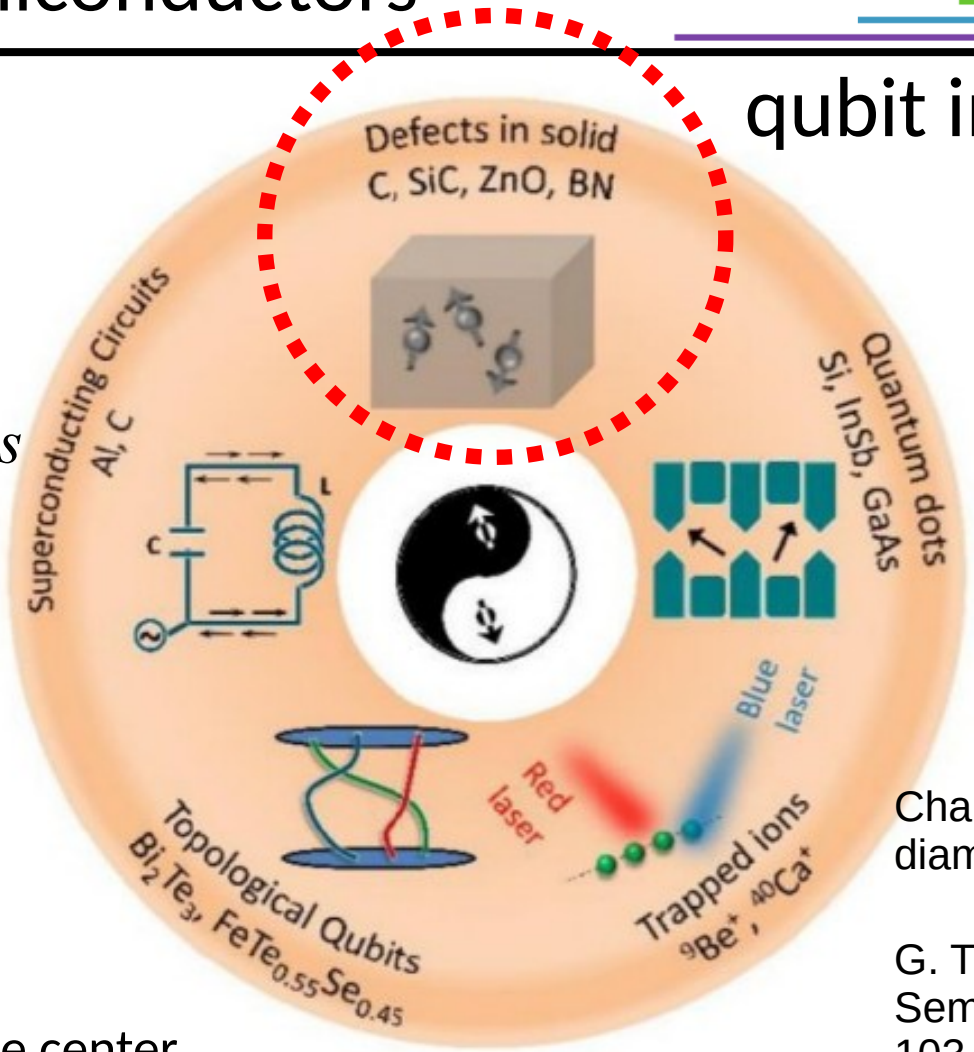
qubit implementations

G4V vacancy
*in **diamond***

In short: XV centers



inversion symmetry at the center



a review of diamond defects:

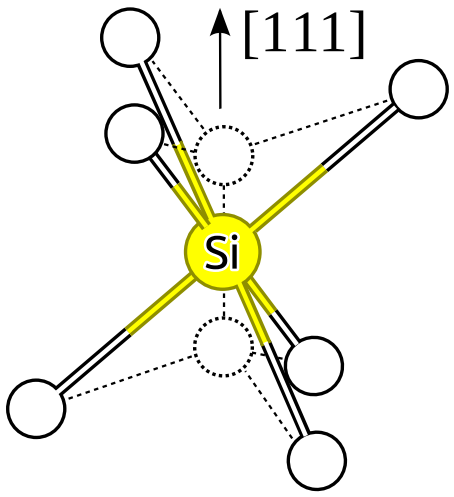
Chapter One - Color centers in diamond for quantum applications

G. Thiering A. Gali
Semiconductors and Semimetal
103 1-36 (2020)

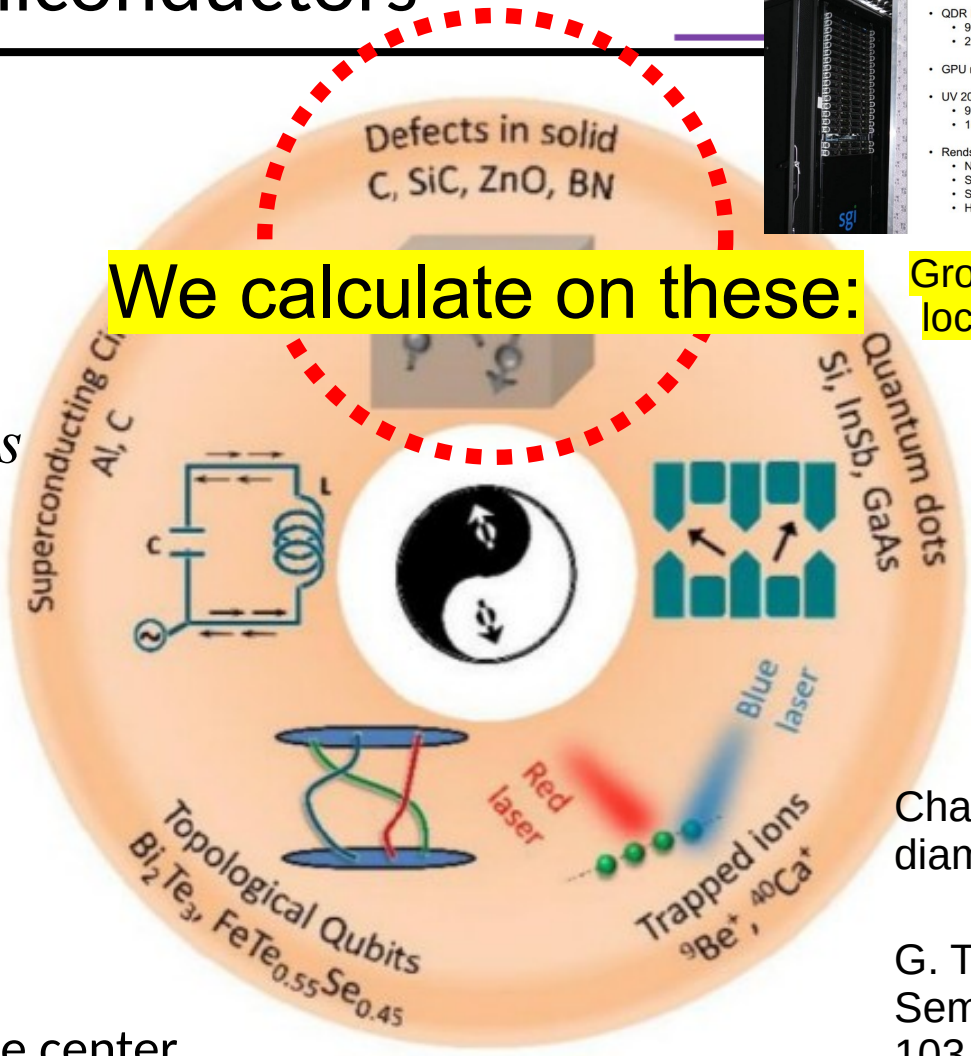
Defects in semiconductors

G4V vacancy
*in **diamond***

In short: XV centers



inversion symmetry at the center



We calculate on these:

Saját számítási infrastruktúra

Konfiguráció:

- QDR InfiniBand cluster:
  - 900 CPU core
  - 2064GB RAM
- GPU node
- UV 2000:
  - 96 CPU core
  - 1024 GB shared memory
- Rendszerszoftverek:
  - Novell SLES 11 operációs rendszer
  - SGI Performance Suite szoftvercsomag
  - SGI Management Center
  - HP Management

nano group Budapest

HPC @hu
Kompetencia Központ

Group's own local cluster

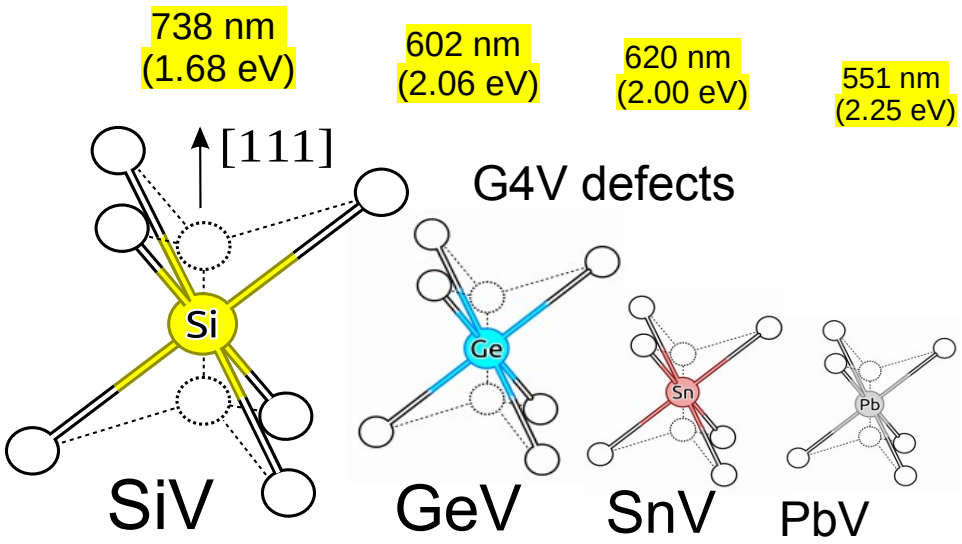
Komondor HPC hungarian suprcomputer

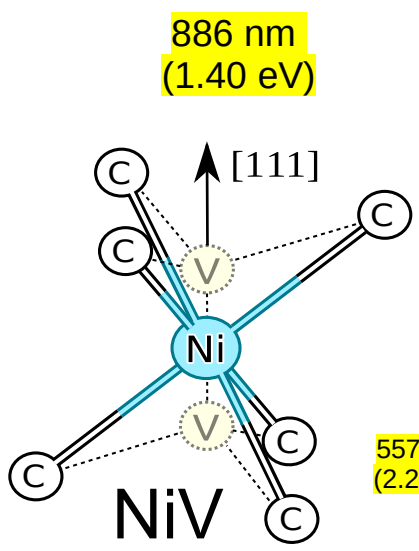
a review of diamond defects:

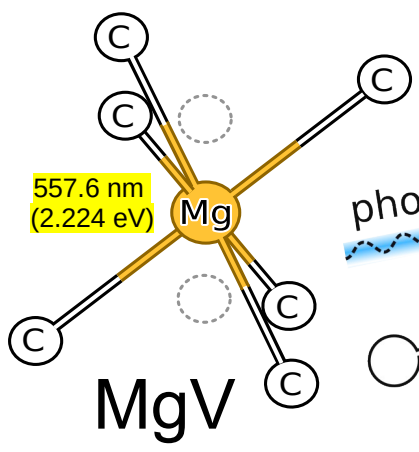
Chapter One - Color centers in diamond for quantum applications

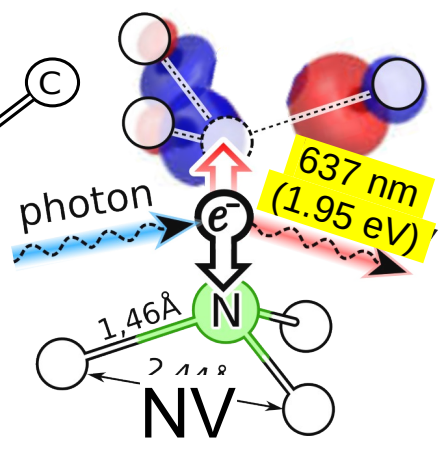
G. Thiering A. Gali
Semiconductors and Semimetal
103 1-36 (2020)

Experimentally observed Qubit candidates in diamond







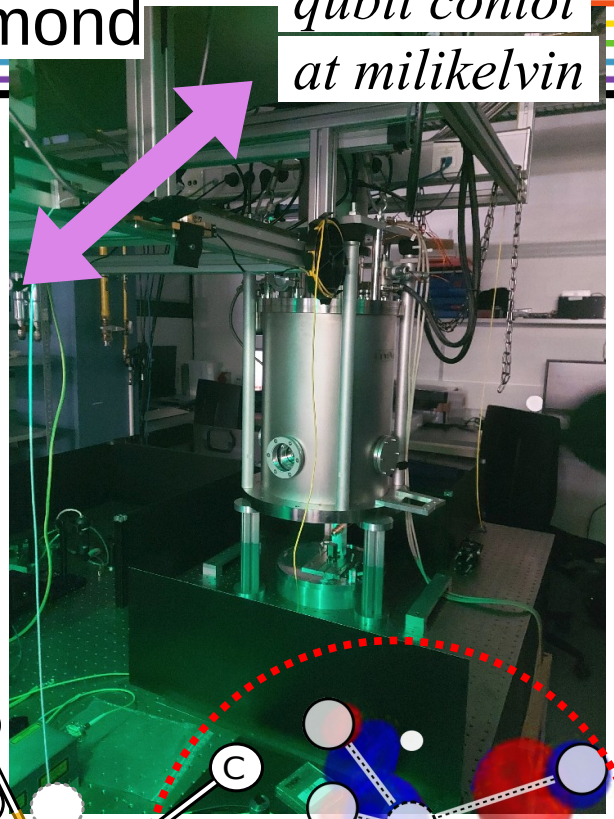


XV(-)'s: G. Thiering and A. Gali Phys. Rev. X **8**, 021063 (2018)
XV(0)'s: G. Thiering and A. Gali npj Comput Mater **5**, 18 (2019)
XV's hyperfine: M Mohseni, L Razinkovas, V Žalandauskas, G Thiering, A Gali arXiv:2408.10407 (2025)

G. Thiering and A. Gali Phys. Rev. Research **3**, 043052 – (2021)

Experimentally observed Qubit candidates in diamond

qubit contol at milikelvin

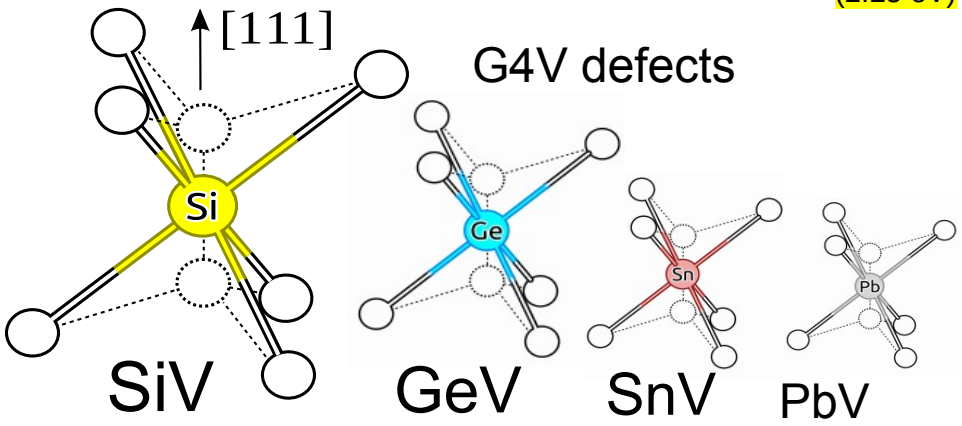


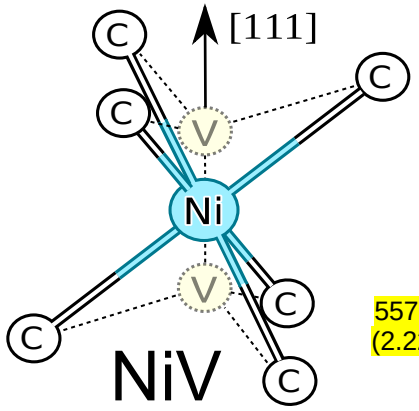
Qubit control via optical lasers: (532 nm green laser)

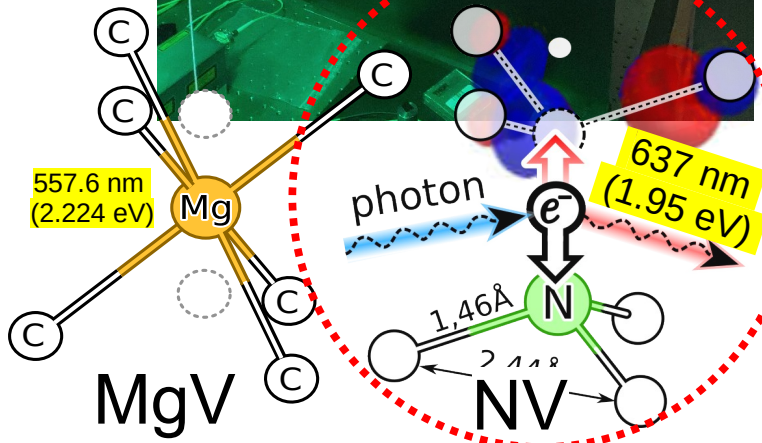
Motivation: determine processes governing T_1, T_2, T_2^*

loss of spin coherence: loss of qubit!

738 nm (1.68 eV) | 602 nm (2.06 eV) | 620 nm (2.00 eV) | 551 nm (2.25 eV) | 886 nm (1.40 eV)





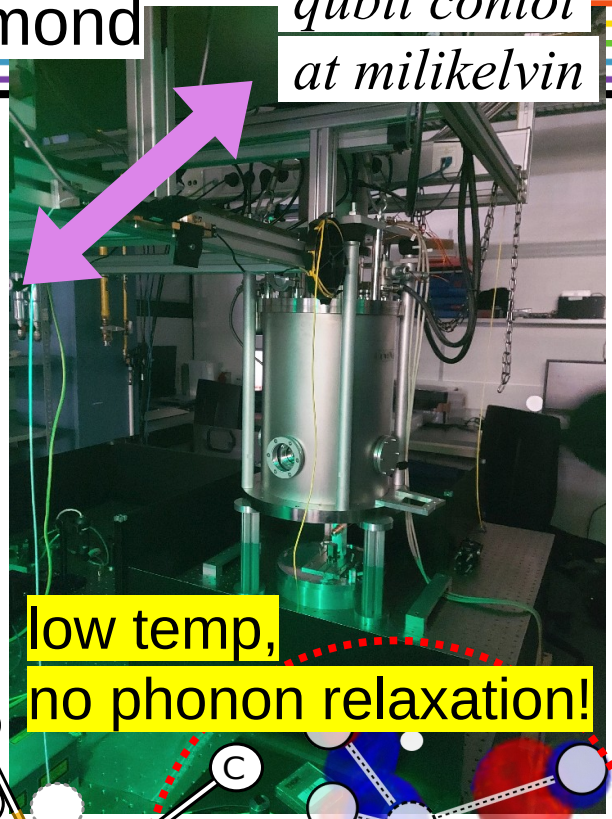


XV(-)'s: G. Thiering and A. Gali Phys. Rev. X **8**, 021063 (2018)
XV(0)'s: G. Thiering and A. Gali npj Comput Mater **5**, 18 (2019)
XV's hyperfine: M Mohseni, L Razinkovas, V Žalandauskas, G Thiering, A Gali arXiv:2408.10407 (2025)

G. Thiering and A. Gali Phys. Rev. Research **3**, 043052 – (2021)

Experimentally observed Qubit candidates in diamond

qubit contol at milikelvin



Qubit control via optical lasers: (532 nm green laser)

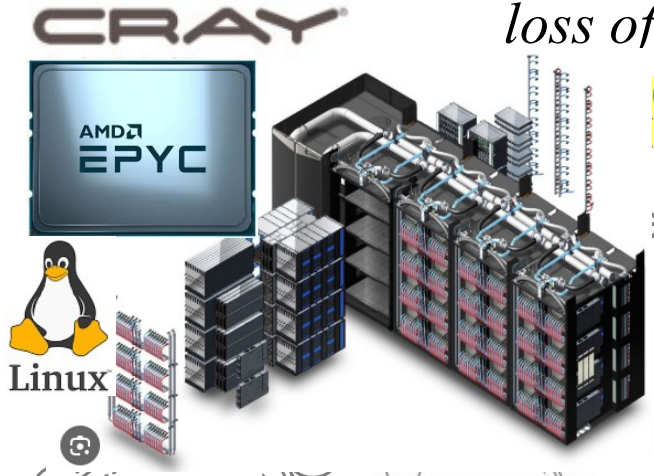
Motivation: determine processes governing T_1, T_2, T_2^*

loss of spin coherence: loss of qubit!

BUT WHY?

Spin-orbit-phonon relaxation

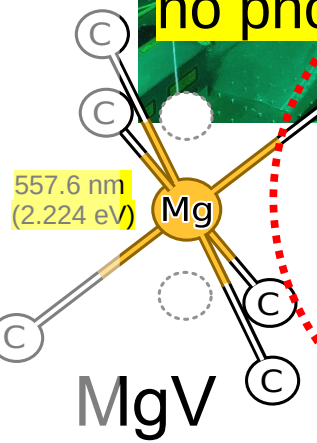
low temp, no phonon relaxation!

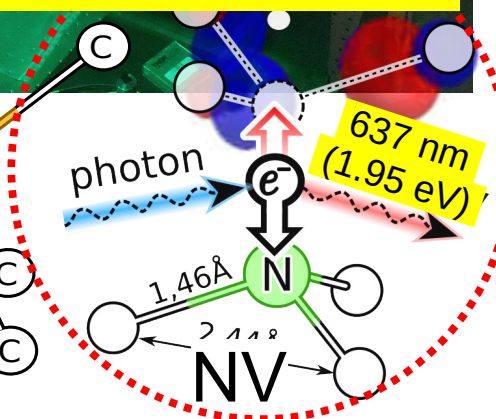


Saját számítási infrastruktúra

lets do HPC computing

(high performance computing)



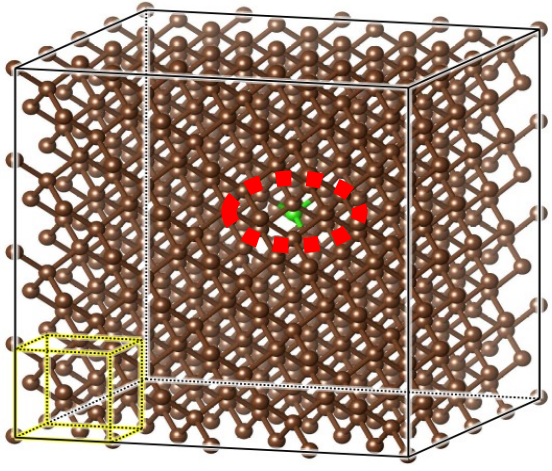


Why *ab-intio* HPC?

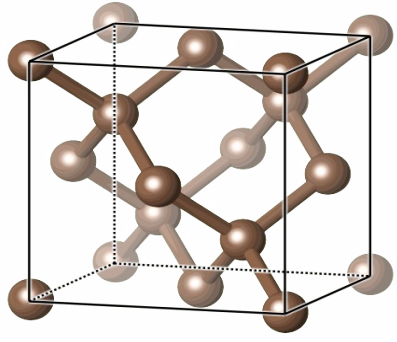
ab-initio package

"DFT" is conventionally used for: electronic structure

simulate defects *in* ~100-1000-atom *supercells to get:*



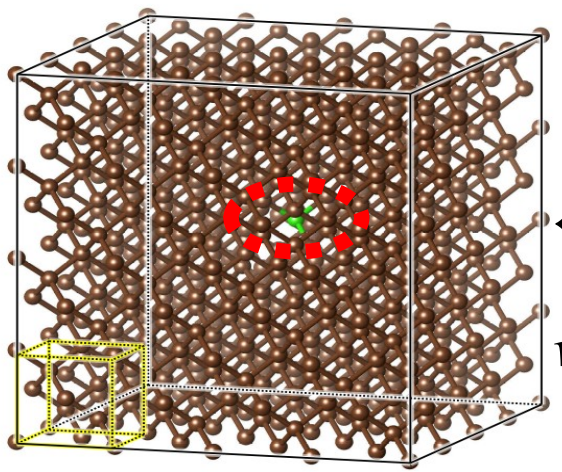
← *512-atom supercell with* **SiV** *inside*



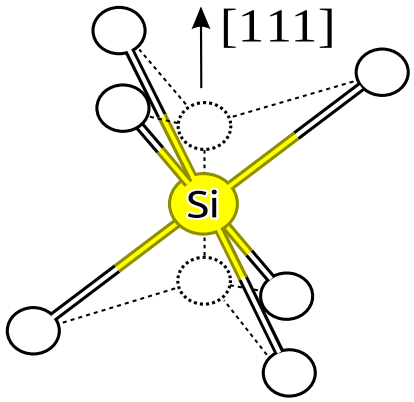
← *diamond Bravais lattice (8-atom supercell)*

"DFT" is conventionally used for: electronic structure

simulate defects *in* ~100-1000-atom *supercells to get:*

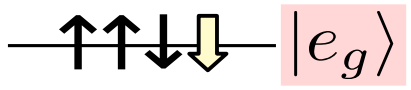


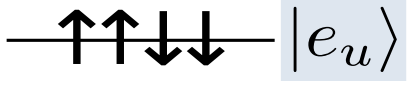
← *512-atom supercell with* **SiV** *inside*

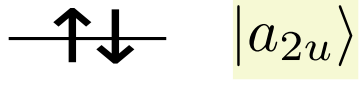


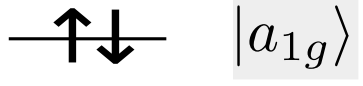
S=1/2 spin

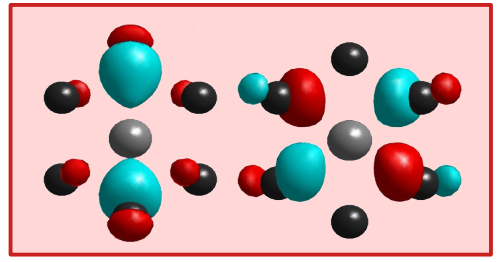
hole

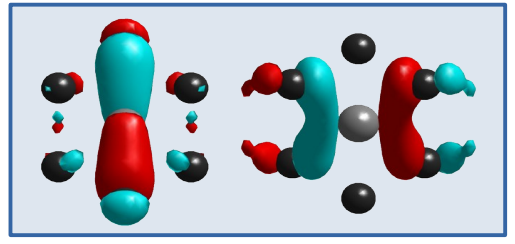


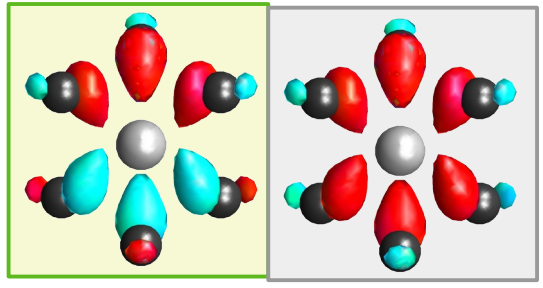












Why *ab-intio* HPC?

VASP b-initio ienna ackage imulation — *ab-initio package*

DFT is conventionally used for: electronic structure

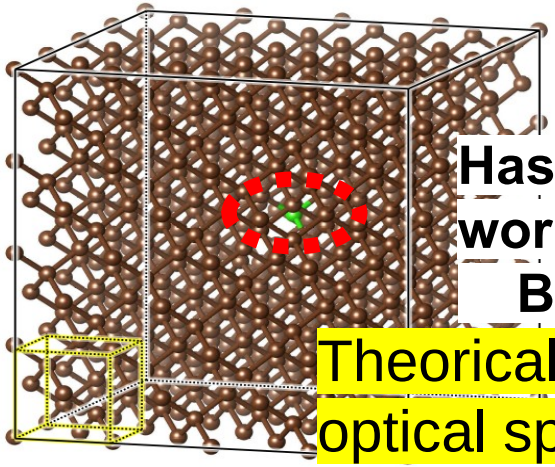
simulate defects in ~100-1000-atom *supercells to get:*

- ☞ **Formation** energies
- ☞ **Optical** excitations (~ 0.1 eV *precision – HSE06 hybrid functional)*
- ☞ **Electron-phonon** coupling *(vibronic sideband for optical centers)*

An exemplary example:

example: 2nd excited state of carbon vacancy in diamond

→ GR1 center

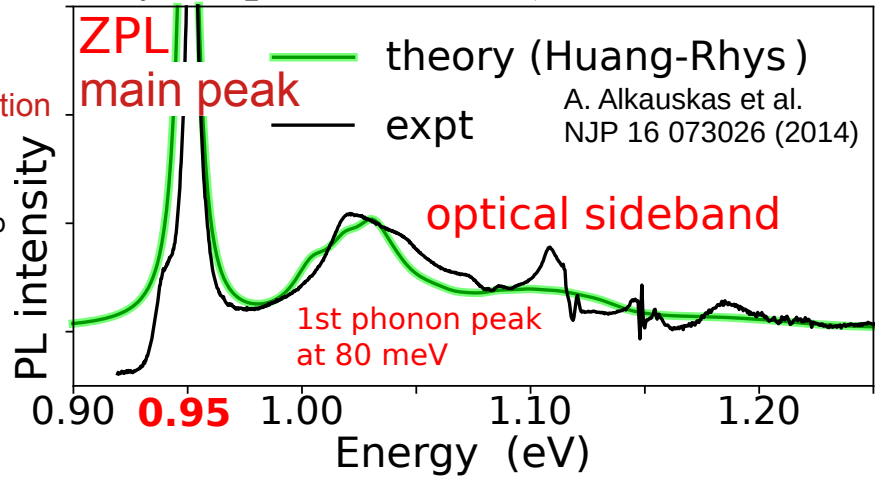


Hasselt diamond workshop
Belgium - (2025)

Theorically predicted optical spetrum

zero-phonon transition

Ronald Ulbricht group
Mainz, Germany



P18 **Transient Absorption Spectroscopy of Carbon Vacancies in Diamond: Electronic Structure and Dynamics** Minh-Tuan Luu

Minh-Tuan Luu,[1] Ali Tayefeh Younesi,[1] Gergő Thiering,[2] Alexandre Zaitsev,[3] and Ronald Ulbricht[1]

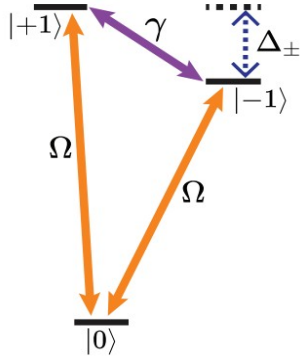
Why *ab-intio* HPC?

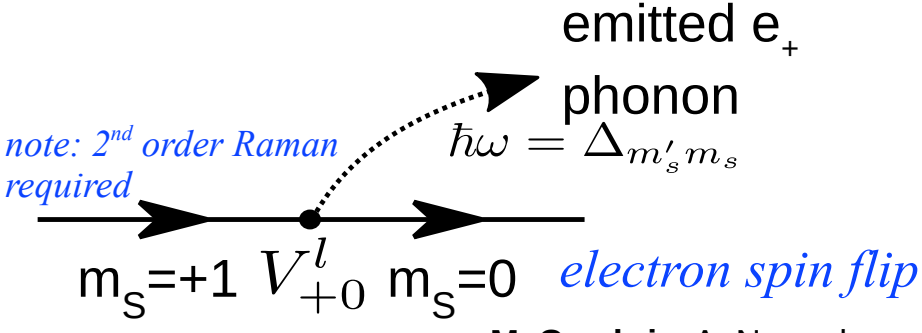
ab-initio package

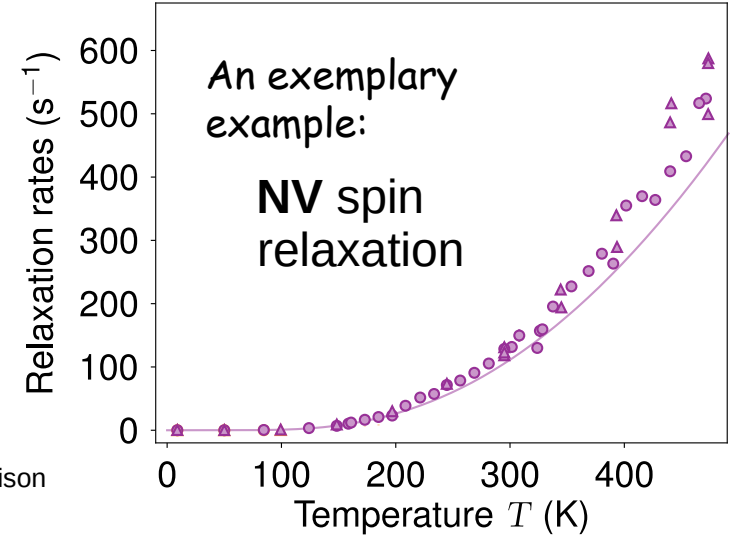
DFT is conventionally used for: electronic structure

simulate defects in ~100-1000-atom *supercells to get:*

- ☞ **Formation** energies
- ☞ **Optical** excitations (~ 0.1 eV *precision – HSE06 hybrid functional)*
- ☞ **Electron-phonon** coupling *(vibronic sideband for optical centers)*
- ☞ **Spin-phonon** interaction *(spin* T_1, T_2, T_2^* *predictions)*







Physical Review Letters
130 (25), 256903 (2023)

M. Cambria, A. Norambuena, H. Dinani, **G. Thiering**, A Gardill, I Kemeny, Y Li, V Lordi, Ádám Gali, JR Maze, **S Kolkowitz**

group @University of Wisconsin, Madison

*lines are **fully ab-initio** predictions, no fit parameters*

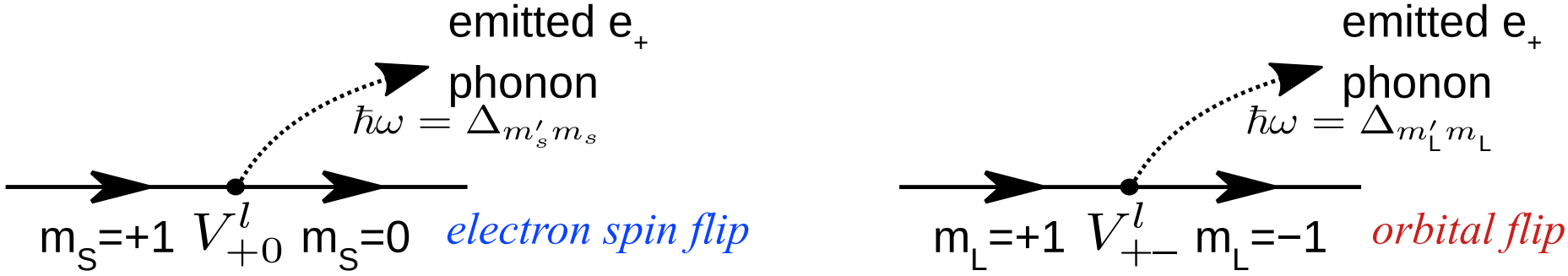
Why *ab-intio* HPC?

VASP b-initio ackage imulation Vienna — *ab-initio package*

DFT is conventionally used for: electronic structure

simulate defects in ~100-1000-atom *supercells to get:*

- ☞ **Formation** energies
- ☞ **Optical** excitations (~ 0.1 eV *precision – HSE06 hybrid functional)*
- ☞ **Electron-phonon** coupling *(vibronic sideband for optical centers)*
- ☞ **Spin-phonon** interaction *(spin* T_1, T_2, T_2^* *predictions)*



aim: *determine unconventional (spin) parameters inaccessible by experiments*

This talk: Predict phonon assisted *spin relaxation* in **SiV** *in diamond*

Why *ab-intio* HPC?

VASP b-initio ienna ackage imulation — *ab-initio package*

DFT is conventionally used for: electronic structure

simulate defects in ~100-1000-atom *supercells to get:*

- ☞ **Formation** energies
- ☞ **Optical** excitations *(~0.1 eV precision – HSE06 hybrid functional)*
- ☞ **Electron-phonon** coupling *(Jahn-Teller effect), (vibronic coupling)*
- ☞ **Spin-phonon** relaxation *(spin* T_1, T_2, T_2^* *predictions)*
- ☞ **Spin-orbit** matrix elements: $\lambda \boldsymbol{LS}$ *(λ up to ~20% precision)*
- ☞ **Spin-spin** interaction: **ZFS** (*Zero field splitting*) *magnetic dipole-dipole:* $\boldsymbol{SDS}$
- ☞ **Hyperfine** interaction: *electronic + nuclear spin dipole-dipole:* $\boldsymbol{SAI}$
- ☞ **Nuclear quadrupolar:** $\boldsymbol{IQI}$

We require:

programming: Python, Fortran etc.

solid state physics + group theory

HUN-REN Hungarian Research Network

Wigner

We offer:

Travel to International Conferences,
Mellékkereset hallgatóknak
Eredmények esetén

Wigner Centre for Physics

Bsc, Msc témakiírás (diploma topics)
https://www.ttk.bme.hu/node/8850

TDK, Bsc, Msc, PhD students are welcome!

Semiconductor nanostructures Research Group

Adam Gali
Gergő Thiering (me)
Anton Pershin
Meysam Mohseni
Nima Ghafaricherati
Bian Guodong
Xiangru Han
Nasrin Estaji
Zoltán Sántha
Balázs Tóth

@Hungary
@Budapest

QUANTERA MAESTRO

KIFÜ
Kifü HPC
Hungary

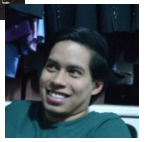
Thank you for your kind attention!

Ulm University (Germany)
Fedor Jelezko
group:
Florian Frank

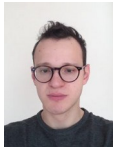
Berndt Koslowski

Katharina Senkalla

City College of New York
Carlos A. Meriles



group:
Richard Monge
Tom Delord



Lukas Razinkovas
Vilnius, FTMC

Ronald Ulbricht
Mainz, Germany

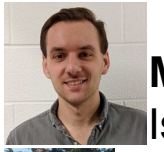
János Bolyai Research Scholarship

NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE
HUNGARY
PROJECT FINANCED FROM THE NRDI FUND
MOMENTUM OF INNOVATION

NKKP STARTING
150113. *Hungary*

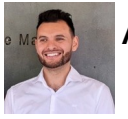
nano group Budapest
wiki.kfki.hu/nano

University of Wisconsin-Madison
Shimon Kolkowitz's
group:



Matt Cambria
Ishita Kemeny
Yanfei Li
Aedan Gardill

Universidad Mayor, Chile
Jeronimo Maze *group*



Ariel Norambuena
Hossein Dinani

Lawrence Nat. lab
Vincenzo Lordi