Computational Materials Science Centers: Midwest Integrated Center for Computational Materials (MICCoM)

Giulia Galli, MICCoM Director
Argonne National Laboratory & University of Chicago

http://miccom-center.org/index.html

BESAC Meeting, July 27th, 2023

Computational Materials Science Centers

https://science.osti.gov/bes/Research/Computational-Materials-and-Chemical-Sciences-CMS-CCS

Computational Materials Sciences (CMS) supports integrated theory-computation-experimental teams to perform the basic research required to deliver **open-source community codes** and the associated experimental and theoretical **databases for predictive design of functional materials** using **current leadership class computers** and **exa-scale platforms.**

- Started Sep 2015 for 4 years
- Renewals Aug 2019 for 4 years
- Renewals Aug 2023 for 3 years

Computational Materials Science Centers

- **MICCoM** - **Argonne National Laboratory** (PI Giulia Galli): Midwest Integrated Center for Computational Material
- **COMSCOPE** - **Brookhaven National Laboratory** (PI Gabriel Kotliar): Center for Computational Materials Science and Design (*strongly correlated materials*)
- **C2SEPEM** - **Lawrence Berkeley National Laboratory** (PI Steven Louie): Center for Computational Study of Excited State Phenomena in Energy Materials
- **NPNEQ** - **Lawrence Livermore National Laboratory** (PI Tadashi Ogitsu): Center for Non-Perturbative Studies of Functional Materials under Non-Equilibrium Conditions
- **CPSFM** - **Oak Ridge National Laboratory** (PI Paul Kent): Center for Predictive Simulation of Functional Materials (*Quantum Monte Carlo [QMC]*)

- **COMMS** - **Pennsylvania State University** (PI Long-Qing Chen) : Computational Mesoscale Science and Open Software for Quantum Materials
- **QMC-HAMM** - **University of Illinois, Urbana-Champaign** (PI David Ceperley) : From accurate correlated quantum simulations to mesoscopic scales *[QMC for ML]*
- **EPW** - **University of Texas, Austin** (PI Feliciano Giustino): Toward Exascale Computing of Electron-Phonon

MICCoM: Midwest Integrated Center for Computational Materials

MICCoM (http://miccom-center.org/) develops and disseminates interoperable computational tools - open source software, data, simulation templates, and validation procedures - that enable simulations and predictions of properties of **materials** for **low-power electronics** and for **quantum technologies**

Lead Institution: Argonne

Participating Institutions:
University of Chicago
University of Notre Dame
University of California Davis
University of Modena&Reggio Emilia, Italy

Program Managers: Matthias Graf and Claudia Mewes

MICCoM: Midwest Integrated Center for Computational Materials

MICCoM (http://miccom-center.org/) develops and disseminates interoperable computational tools - open source software, data, simulation templates, and validation procedures - that enable simulations and predictions of properties of **materials** for **low-power electronics** and for **quantum technologies**

MICCoM Team

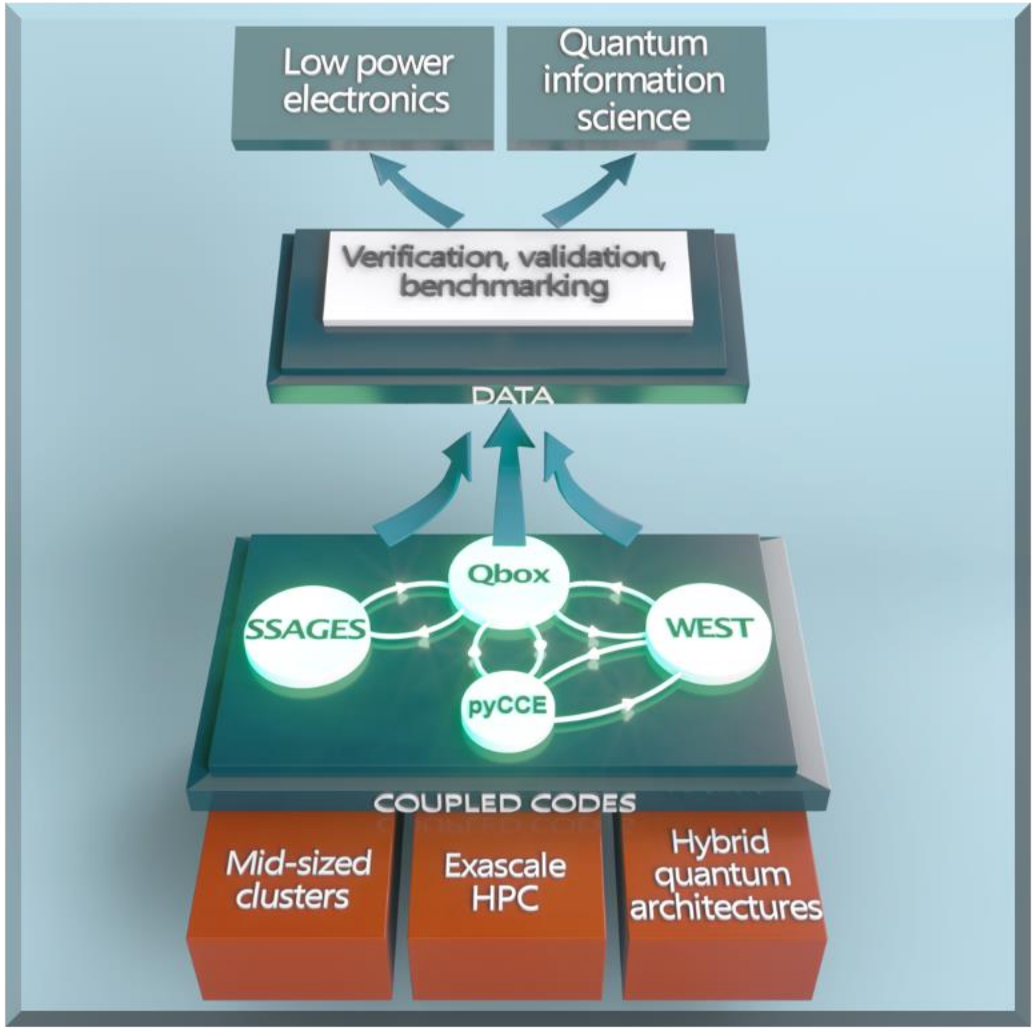
MICCoM: Midwest Integrated Center for Computational Materials

Distinctive features of the center:

•Development of **interoperable codes** for simulation of materials at multiple length and time scales

•Focus on **heterogeneous materials**, including defects, interfaces, and building blocks

•Focus on **spectroscopic** and **coherence properties**



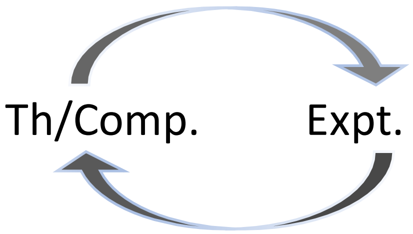
Some guiding principles

- Scientific innovation requires **sustained method & algorithmic developments**, in addition to improving accuracy and range of applicability of existing ones.

- **Coupling** of **methods** and of **codes**, including between different centers, is required to target **multiple properties** of **heterogeneous materials** and for software **sustainability.**

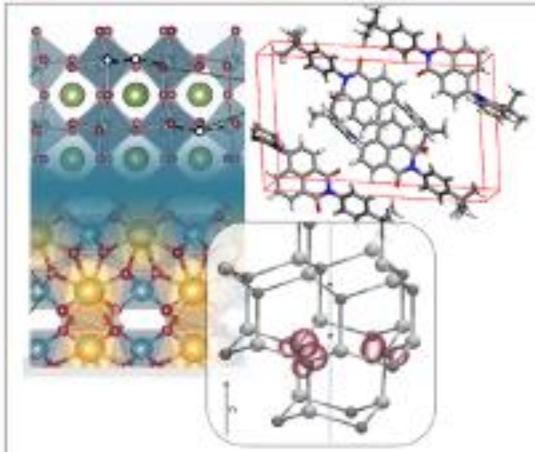
- **Exascale is one, albeit not the only scale:** successful computational strategies are hybrid and require software running on multiple architectures, including quantum computers.

- **Integration with experiments** is key and not a given.

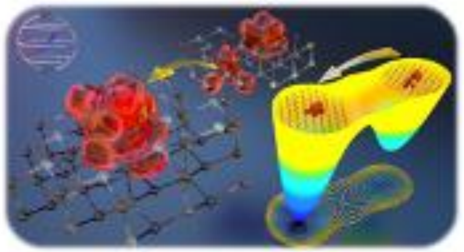


- Making computational **data robust** (reproducible, w/margin of errors) and **available** is critical for the success of simulations and an increasingly pressing need in the age of AI/ML.

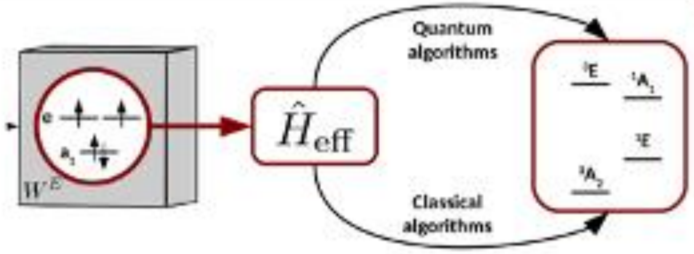
Multiple properties of heterogeneous systems



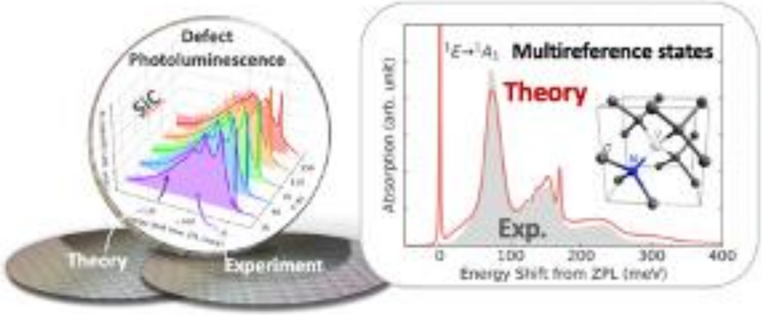
Electronic properties of weakly correlated materials at zero and finite T



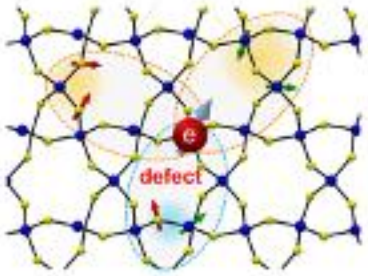
Free energy surfaces and dynamical properties



Electronic properties of strongly correlated regions

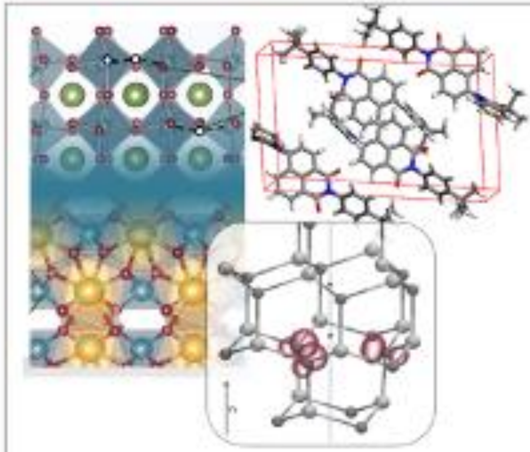


Optical properties



Spin and coherence properties

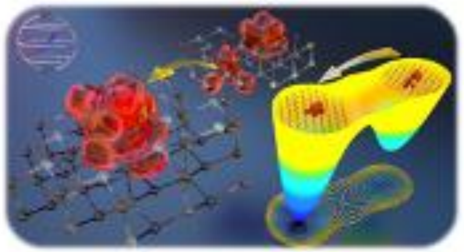
Multiple methods and algorithms



Electronic properties of weakly correlated materials at zero and finite T

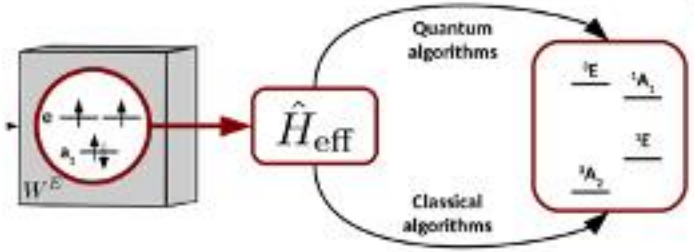
DFT & hybrid DFT and Many Body Perturbation Theory (GW)

First Principles Molecular Dynamics



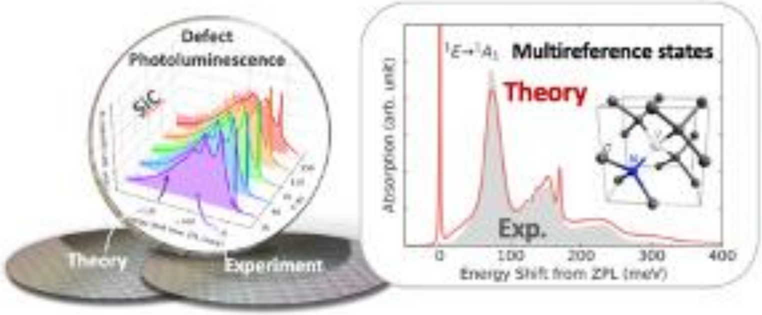
Free energy surfaces and dynamical properties

Advanced sampling including w/quantum forces for ground & excited states



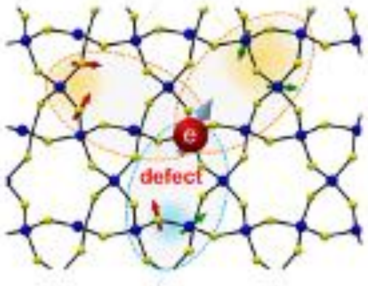
Electronic properties of strongly correlated regions

Quantum Embedding Theories: QDET and embedded BSE



Optical properties

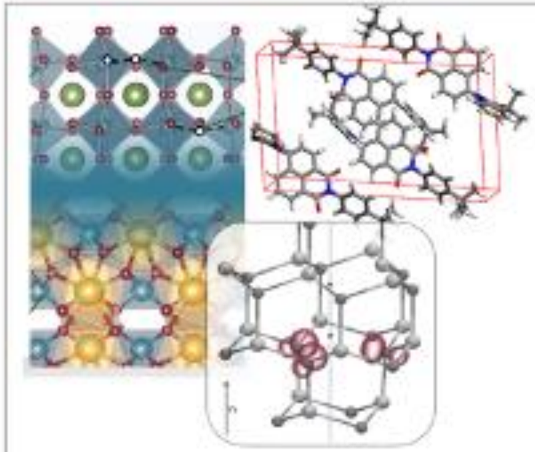
(Spin-flip) Time Dependent DFT, w/forces, and BSE



Spin and coherence properties

Spin Hamiltonians with ab initio parameters and CCE techniques

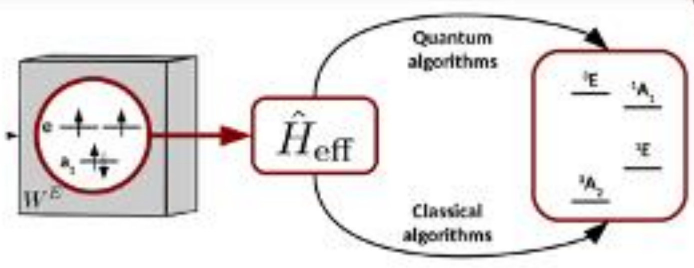
Multiple, coupled codes



Electronic properties of weakly correlated materials at zero and finite T

DFT & hybrid DFT *[Qbox & QE]* and Many Body Perturbation Theory (GW)

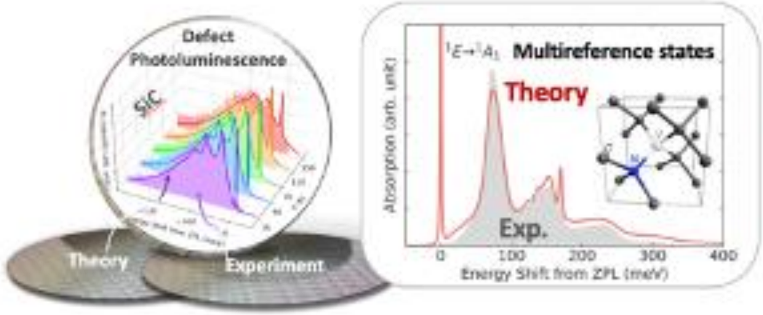
First Principles Molecular Dynamics *[Qbox]*



Electronic properties of strongly correlated regions

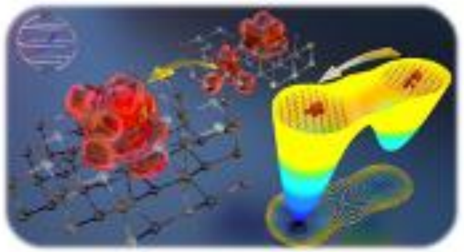
Quantum Embedding Theories: QDET and embedded BSE

[QE, WEST & pySCF]



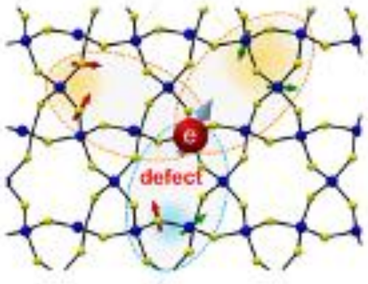
Optical properties

(Spin-flip) Time Dependent DFT, w/forces, and BSE *[WEST]*



Free energy surfaces and dynamical properties

Advanced sampling including w/quantum forces for ground & excited states *[Qbox-SSAGES & Qbox-i-PI]*



Spin and coherence properties

Spin Hamiltonians with ab initio parameters *[QE]* and CCE techniques *[pyCCE]*

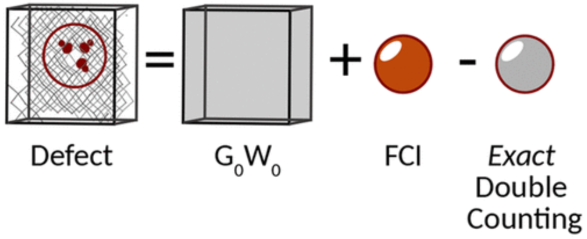
MICCoM-enabled software innovation: example

When it all comes together: Quantum embedding for **highly correlated defects** developed, code optimized, released to the community, and prepared for exascale in ~ 1 year

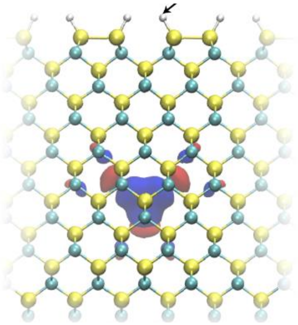
- **Method published** — 06/2022
- **Code released (CPU & GPU)** — 09/2022
- **Taught in MICCoM school** — 10/2022
- **Online tutorials released** — 01/2023
- **Code prepared for exascale** — Spring 2023

Code installed also on: NERSC/Perlmutter, OLCF/Summit, ALCF/Theta

Sheng, Vorwerk, Govoni, Galli, J. Chem. Theory Comput. 18, 3512 (2022) & Nature Comp. Scie. 2022



Many-body states of defects **in bulk**



Many-body states of defects **close to surfaces**

MICCoM-enabled methodological advances

The full realization of spin qubits for quantum technologies relies on the ability to control and design the formation processes of spin defects in semiconductors and insulators:

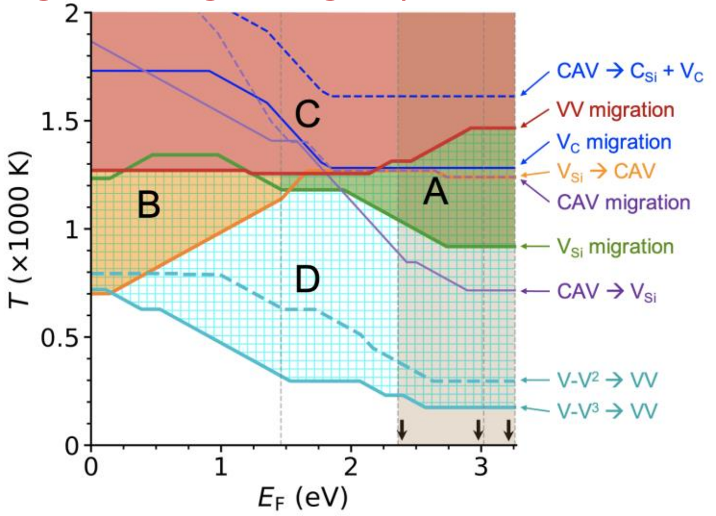
How do defects form? How can we design and control them?

We devised a computational protocol to investigate the **synthesis of point-defects** at the atomistic level and studied a promising spin-qubit in silicon carbide.

We **combined** methods & codes:

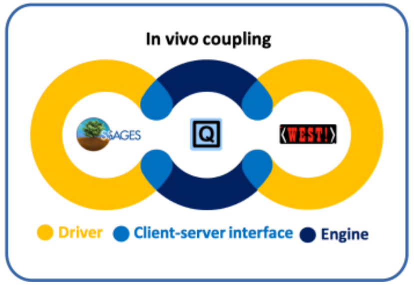
- First principles MD (Qbox) & advanced sampling (SSAGES & PySAGES) to compute activation temperatures and barriers at finite T.
- High-level electronic structure calculations (WEST: from GW, TDDFT to QDET) on first principle MD trajectories

Design rules guiding experiments

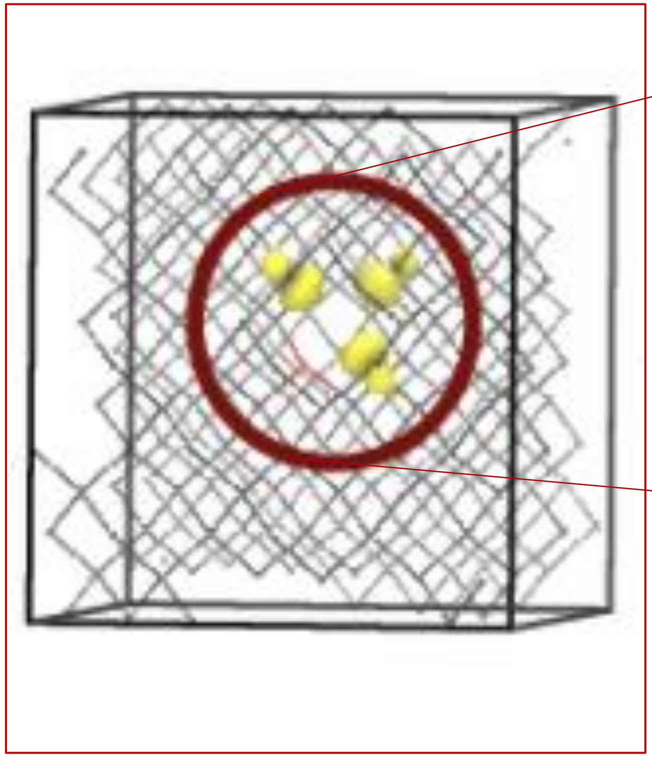


E. Lee, J. De Pablo, G.Galli, Nat. Comm. 2021; C.Zhang, F.Gygi and G.Galli Nat. Comm. (under review)

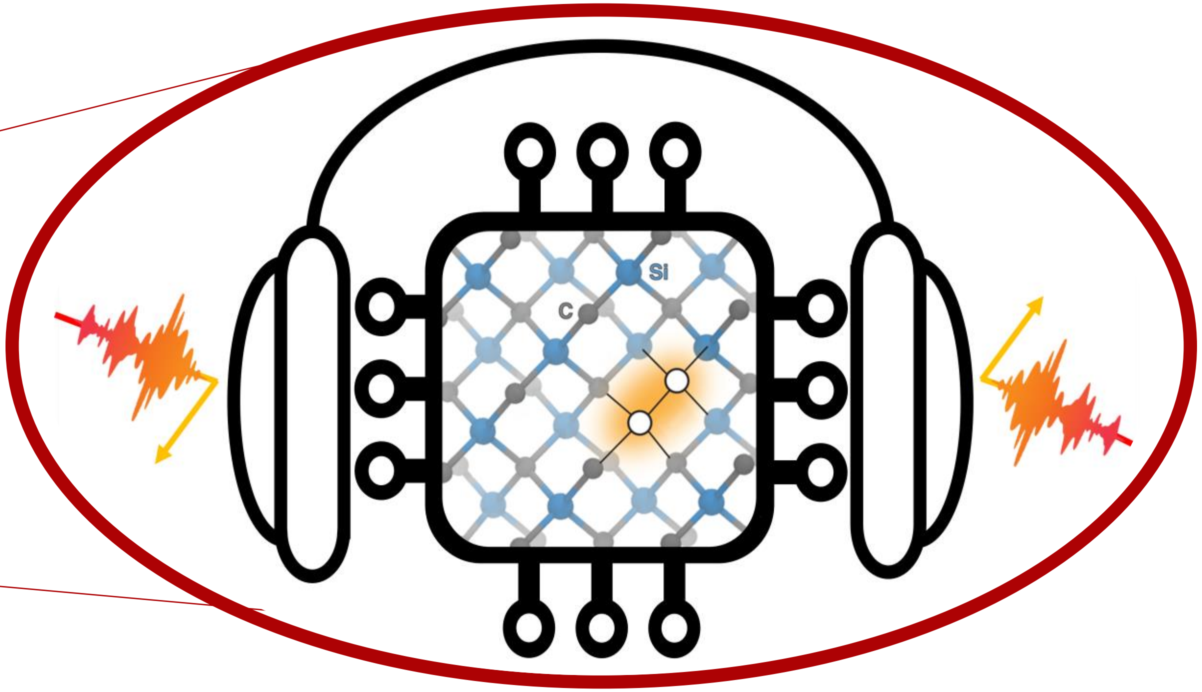
M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, G. Galli, npj Comp Mat 2021; Emre Sevgen et al. JCTC 2018



Solved the electronic structure of point defects on NISQ computers (Noisy Intermediate Scale Quantum Computers)



B.Huang, M.Govoni, GG PRX-Q 2022 & JCTC 2023



Results on quantum hardware (IBM Casablanca & Guadalupe through ORNL) with noise *cancellation*

Data strategy: bring published papers to "life"

- Make available, in a **decentralized, distributed** manner, all **data** and **procedures** presented in scientific papers.

M.Govoni, G.Galli, J.J.de Pablo et al. Scientific Data 2019

- The **Qresp** package facilitates:
  - **organization of data** presented in scientific papers
  - **succinct description** of the experimental and/or computational procedures
  - **generation of searchable metadata**

It has been a struggle …

Community engagement and impact of collaborations

National Labs

- **NIST** (WEST, SSAGES)
- **LBNL** (Qbox)
- **LLNL** (Qbox)
- **APS@ANL** (Qbox)

EFRCs (ALL codes)

- **AMEWS** (ANL)
- **NPQC** (LBL/ANL)
- **QMEENC** (UCSD)
- **CHOISE** (NREL)

Innovation Hub

(ALL codes)

- **Q-NEXT** (ANL)

MICCoM

Nat'l Collab.

- **CCSC-CSI**
- **DOE/SunRISE** (Qbox,WEST)
- **NSF/MRSEC** (ALL codes)
- **NSF/Duke** (Qresp)
- **AFOSR&ONR** (Qbox, WEST, PyCCE)
- **Boeing** (WEST)

Target of Opportunity Projects (TOPs)

- **T.Berkelbach** (WEST)
- **V.Gavini**(PyCCE)
- **B.Roux** (SSAGES)
- **A.Ferguson** SSAGES/CoPPS)

Int'l Collab.

- **IBM-UK/Daresbury** (SSAGES)
- **DTU** (Denmark) (SSAGES, Qbox)
- **Osaka Univ.** (WEST)

MICCoM: Summary

- A sustained innovation factory for new methods and new strategies to solve materials problems while providing exemplary open-source software to the community
- A proponent of new, coupled simulation strategies on hybrid architectures, including quantum computers
- A center for the stewardship of (FP)MD & MBPT reference data and open papers