***Partners in crime* for ten years**

… and counting

Davis, 2013


Davis, 2013


Davis, 2013

Chicago, 2014 →


Young Building, 2014


Chicago, 2015
MICCoM
Midwest Integrated Center
for Computational Materials

We published ~ 40 papers together

Large scale GW calculations, Marco Govoni and Giulia Galli, J. Chem. Theory Comput. 11, 2680 (2015)

1st release of WEST when we submitted the first MICCoM proposal

1. Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli, J. Chem. Theory Comput. Accepted (2023).
2. Roadmap on Electronic Structure Codes in the Exascale Era, V. Gavini, ... , G. Galli, M. Govoni, F. Gygi et al., Submitted (2022). arXiv:2209.12747
3. Vibrationally resolved optical excitations of the nitrogen-vacancy center in diamond, Yu Jin, Marco Govoni, and Giulia Galli, npj Comput. Mater. 8, 238 (2022).
4. Computational protocol to evaluate electron-phonon interactions within density matrix perturbation theory, Han Yang, Marco Govoni, Arpan Kundu, and Giulia Galli, J. Chem. Theory Comput. 18, 6031 (2022).
5. Green's function formulation of quantum defect embedding theory, Nan Sheng*, Christian Vorwerk*, Marco Govoni, and Giulia Galli (*equal contribution), J. Chem. Theory Comput. 18, 3512 (2022).
6. Simulating the electronic structure of spin defects on quantum computers, Benchen Huang, Marco Govoni, and Giulia Galli, PRX Quantum 3, 010339 (2022).
7. Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers, Christian Vorwerk*, Nan Sheng*, Marco Govoni, Benchen Huang, and Giulia Galli (*equal contribution), Nat. Comput. Sci. 2, 424 (2022).
8. Combined first-principles calculations of electron-electron and electron-phonon self-energies in condensed systems, Han Yang, Marco Govoni, Arpan Kundu and Giulia Galli, J. Chem. Theory Comput. 17, 7468-7476 (2021).
9. Photoluminescence spectra of point defects in semiconductors: Validation of first principles calculations, Yu Jin, Marco Govoni, Gary Wolfowicz, Sean E. Sullivan, F. Joseph Heremans, David D. Awschalom and Giulia Galli, Phys. Rev. Mater. 5, 084603 (2021).
10. Quantum Vibronic Effects on the Electronic Properties of Solid and Molecular Carbon, Arpan Kundu, Marco Govoni, Han Yang, Michele Ceriotti, Francois Gygi, and Giulia Galli, Phys. Rev. Mat. Letters 5, L070801 (2021).
11. Quantum Embedding Theory for Strongly-correlated States in Materials, He Ma, Nan Sheng, Marco Govoni and Giulia Galli, J. Chem. Theory Comput. 17, 2116-2125 (2021).
12. Machine Learning Dielectric Screening for the Simulation of Excited State Properties of Molecules and Materials, Sijia Dong, Marco Govoni and Giulia Galli, Chem. Sci. 12, 4970-4980 (2021).
13. Code interoperability extends the scope of quantum simulations, Marco Govoni, Jonathan Whitmer, Juan de Pablo, Francois Gygi, Giulia Galli, Npj Comput. Mater. 7, 32 (2021). 10.1038/s41524-021-00501-z
14. First-principles Studies of Strongly Correlated States in Defect Spin Qubits in Diamond, Ma He, Nan Sheng, Marco Govoni and Giulia Galli, Physical Chemistry Chemical Physics, (2020). 10.1039/D0CP04585C
15. Quantum simulations of materials on near-term quantum computers, He Ma, Marco Govoni and Giulia Galli, npj, Comput. Mat., 6 (85), (2020). 10.1038/s41524-020-00353-z
16. PyCDFT: A Python package for constrained density functional theory, He Ma, Wennie Wang, Siyoung Kim, Man-Hin Cheng, Marco Govoni and Giulia Galli, J. Comp. Chem., 41, 1859 (2020). 10.1002/JCC.26354
17. PyZFS: A Python package for first-principles calculations of zero-field splitting tensors, He Ma, Marco Govoni and Giulia Galli. J. Open Source Softw., 5(47), 2160 (2020). 10.21105/joss.02160.

18. Discovery, Design, and Dissemination, Raul Laasner, Xiaochen Du, Aditya Tanikanti, Connor Clayton, Marco Govoni, Giulia Galli, Matti Ropo and Volker Blum, J. Open Source Software, 5(45), 1945 (2020). 10.21105/joss.01945
19. Improving the efficiency of G0W0 calculations with approximate spectral decompositions of dielectric matrices, Han Yang, Marco Govoni and Giulia Galli, J. Chem. Phys. 151, 224102 (2019). 10.1063/1.5126214
20. Dielectric-dependent hybrid functionals for heterogeneous materials, Huihuo Zheng, Marco Govoni and Giulia Galli, Phys. Rev. Mat. 3, 073803 (2019). 10.1103/PhysRevMaterials.3.073803
21. Finite-field approach to solving the Bethe-Salpeter equation, Ngoc Linh Nguyen, He Ma, Marco Govoni, Francois Gygi and Giulia Galli, Phys. Rev. Lett. 122, 237402 (2019). 10.1103/PhysRevLett.122.237402
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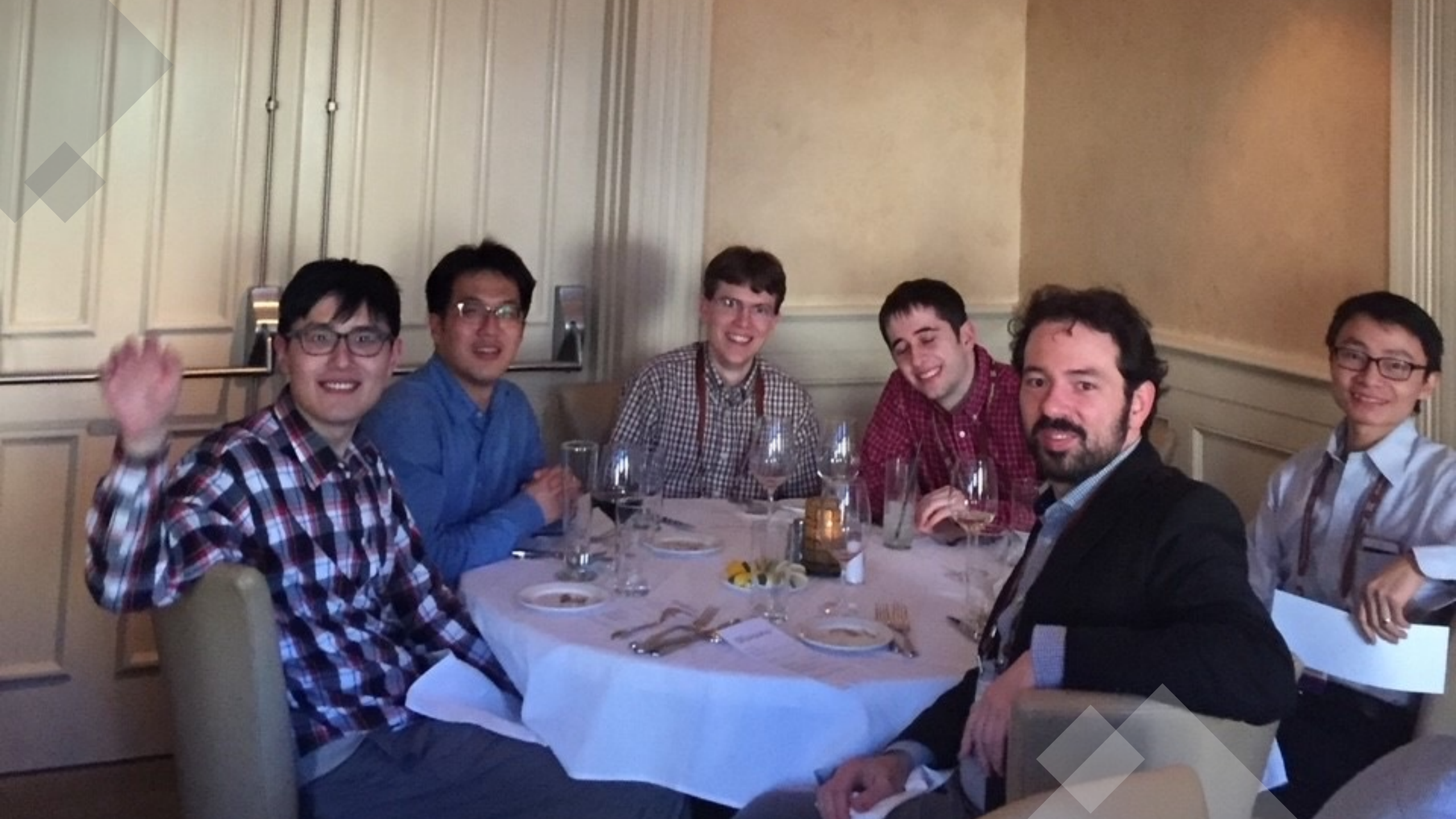
23. A Finite-field Approach for GW Calculations Beyond the Random Phase Approximation, He Ma, Marco Govoni, Francois Gygi and Giulia Galli, J. Chem. Theory. Comp., 15 (1), 154-164 (2019). 10.1021/acs.jctc.8b00864
24. Coupling First Principles Calculations of Electron-Electron and Electron-Phonon Scattering, and Applications to Carbon-based Nanostructures, Ryan L. McAvoy, Marco Govoni, and Giulia Galli, J. Chem. Theory. Comp., 14 (12), 6269-6275 (2018). 10.1021/acs.jctc.8b00728
25. The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers, Matteo Gerosa, Francois Gygi, Marco Govoni and Giulia Galli, Nature Materials, 17, 1122-1127 (2018). 10.1038/s41563-018-0192-4
26. Dielectric Properties of Condensed Systems Composed of Fragments, Ding Pan, Marco Govoni, and Giulia Galli, J. Chem. Phys., 149, 051101 (2018). 10.1063/1.5044636
27. GW100: Comparison of methods and accuracy of results obtained with the WEST code, Marco Govoni and Giulia Galli, J. Chem. Theory. Comp., 14(4), 1895-1909 (2018). 10.1021/acs.jctc.7b00952
28. Electron affinity of liquid water, Alex Gaiduk, T. Anh Pham, Marco Govoni, Francesco Paesani and Giulia Galli, Nature Comm., 9, 247 (2018). 10.1038/s41467-017-02673-z
29. Designing defect-based qubit candidates in wide-gap binary semiconductors for solid-state quantum technologies, Hosung Seo, He Ma, Marco Govoni, and Giulia Galli, Phys. Rev. Mat 1, 075002 (2017). 10.1103/PhysRevMaterials.1.075002
30. Performance and self-consistency of the generalized dielectric dependent hybrid functional, Nicholas P. Brawand, Marco Govoni, Márton Vörös, and Giulia Galli, J. Chem. Theory Comput. 13, 3318 (2017). 10.1021/acs.jctc.7b00368
31. Electronic Structure of Aqueous Solutions: Bridging the Gap Between Theory and Experiments, Tuan Anh Pham, Marco Govoni, Robert Seidel, Stephen E. Bradforth, Eric Schwegler, and Giulia Galli, Science Advances 3 (6), 1603210 (2017). 10.1126/sciadv.1603210
32. Generalization of dielectric dependent hybrid functionals to finite systems, Nicholas Brawand, Márton Vörös, Marco Govoni, and Giulia Galli, Phys. Rev. X 6, 041002 (2016)
33. Implementation and Validation of Fully-Relativistic GW Calculations: Spin-Orbit Coupling in Molecules, Nanocrystals and Solids, Peter Scherpelz, Marco Govoni, Ikutaro Hamada, and Giulia Galli, J. Chem. Theory Comput. 12 (8), 3523-3544 (2016)
34. Nonempirical range-separated hybrid functionals for solids and molecules, Jonathan Skone, Marco Govoni, and Giulia Galli, Phys. Rev. B 93, 235106 (2016)
35. Photoelectron spectra of aqueous solutions from first principles, Alex P. Gaiduk, Marco Govoni, Robert Seidel, Jonathan Skone, Bernd Winter, and Giulia Galli, J. Am. Chem. Soc. Comm. 138, 6912 (2016)
36. Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies, Hosung Seo, Marco Govoni, and Giulia Galli, Sci. Rep. 6, 20803 (2016)
37. Large scale GW calculations, Marco Govoni and Giulia Galli, J. Chem. Theory Comput. 11, 2680 (2015)
38. Self-consistent hybrid functional for condensed systems, Jonathan H. Skone, Marco Govoni, and Giulia Galli, Phys. Rev. B 89, 195112 (2014)


2016-2017: Watching
Ikutaro dancing..



MICCoM

Midwest Integrated Center for Computational Materials

2017

The Midwest Integrated Center for Computational Materials (**MICCoM**) develops and disseminates interoperable computational tools - open source software, data, simulation templates, and validation procedures - that enable simulations and predictions of properties of **functional materials** for energy conversion and of solid-state materials for quantum information science. The distinctive features of the center are:

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

Denver,
February 2020

Dr. Marco Govoni awarded DOE Early Career Award

Galli Group staff scientist Marco Govoni has been awarded the prestigious Early Career Award from the BES Theoretical Condensed Matter Physics Program. Congratulations, Marco!

Argonne, National Laboratory, 2020

Dr. Marco Govoni awarded tenure (11/10/2021)

Dr. Marco Govoni has just been promoted from Assistant Scientist to Scientist (tenured position) at Argonne National Laboratory. Marco serves as co-PI of the Midwest Integrated Center for Computational Materials (MICCoM). He is the lead developer of the WEST code and is the PI of a DOE Early Career Grant.


The Galli Group
2021


ERC, 2019
University of Chicago


2020


Young, 2014


ERC, 2016


ERC, 2018


The Quad, 2015


ERC, 2017


The GALLI GROUP
@ The University of Chicago
UCHICAGO

Looking forward to Zoom Meetings before the summer and to having you back this summer!

We wish you all the best in your new position

Thanks for everything!!!