Marco Govoni

Associate Professor

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Academic Appointments

July 2024 – present **Associate Professor**, *Dept. of Physics, Computer Science, Mathematics, University of Modena and Reggio Emilia, Modena, Italy*.

March 2023 – June 2024 **Assistant Professor**, *(RTDb) Dept. of Physics, Computer Science, Mathematics, University of Modena and Reggio Emilia, Modena, Italy*.

Nov 2021 – March 2023 **Scientist**, *(tenured researcher) Materials Science Division & Center for Molecular Engineering, Argonne National Laboratory, Lemont IL, USA*.

June 2017 – Oct 2021 **Assistant Scientist**, *(tenure-track researcher) Materials Science Division & Center for Molecular Engineering, Argonne National Laboratory, Lemont IL, USA*.

June 2016 – Oct 2017 **Assistant Scientist-temp**, *(fixed-term researcher) Materials Science Division & Center for Molecular Engineering, Argonne National Laboratory, Lemont IL, USA*.

March 2023 – June 2023 **Instructor**, *(teaching appointment) Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

March 2022 – June 2022 **Instructor**, *(teaching appointment) Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

Jan 2021 – March 2021 **Instructor**, *(teaching appointment) Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

March 2020 – June 2020 **Instructor**, *(teaching appointment) Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

Visiting Appointments

March 2023 – present **Visiting Scientist**, *Materials Science Division, Argonne National Laboratory, Lemont IL, USA*.

March 2023 – present **Visiting Scientist**, *CNR-Nano Institute of Nanoscience, Modena, Italy*.

May 2018 – March 2023 **Visiting Scientist**, *Consortium for Advanced Science and Engineering & Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

Education

Mar 2015 – Sept 2016 **Postdoctoral Researcher**, *Materials Science Division & Center for Molecular Engineering, Argonne National Laboratory, Lemont IL, USA*.

Feb 2014 – Mar 2015 **Postdoctoral Researcher**, *Pritzker School of Molecular Engineering, University of Chicago, Chicago IL, USA*.

Jun 2012 – Feb 2014 **Postdoctoral Researcher**, *Dept. of Chemistry, University of California Davis, USA*.

Feb 2012 – Feb 2013 **Postdoctoral Fellow**, *Italian Leadership Class Computing Facility CINECA, Casalecchio di Reno, Italy; and Dept. of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, Italy*.

Jan 2009 – Feb 2012 **Ph.D. Nanoscience and Nanotechnology**, *University of Modena and Reggio Emilia, Italy*.
Thesis: *"Coulomb-driven recombinations in semiconductors: from bulk to nanocrystals"*. Advisors: Prof. S. Ossicini and Dr. I. Marri.

2006–2008 **M.Sc. Physics**, *University of Modena and Reggio Emilia, Italy*.
Grade: 110/110 with honors. Thesis: *"Role and applications of the vacuum force in microscopic systems"*. Advisor: Prof. C. Calandra Buonaura.

2003–2006 **B.Sc. Physics**, *University of Modena and Reggio Emilia, Italy*.
Grade: 110/110 with honors. Thesis: *"Ab-initio simulations of STM images"*. Advisors: Prof. G. Goldoni, Dr. A. Calzolari, Dr. C. Cavazzoni.

Awards and Fellowships

2024-2029 FIS (Fondo Italiano per la Scienza) Starting Grant in Condensed Matter Physics (ERC panel: PE3).

2020 DOE Early Career Award from the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Theoretical Condensed Matter Physics program.

2016 Japan Society for the Promotion of Science (JSPS) invitation fellowship.

2015 Best Scalable Software Award, Mind the Bytes, University of Chicago.

2012 ISCRA fellowship, awarded by the Italian Leadership Class Computing Facility CINECA.

Qualification Certificates

Quantum computing IBM Qiskit Advocate (https://qiskit.org/advocates/). IBM Certified Associate Developer - Quantum Computation using Qiskit v0.2X. Obtained in June 2022.

ASN for full professorship Italian scientific qualification as full professor in Theoretical Condensed Matter Physics (*Abilitazione Scientifica Nazionale*, 02/B2 sector; *prima fascia*). Released by the Italian Minister for University and Research. Validity: 2022–2031.

ASN for associate professorship Italian scientific qualification as associate professor in Theoretical Condensed Matter Physics (*Abilitazione Scientifica Nazionale*, 02/B2 sector; *seconda fascia*). Released by the Italian Minister for University and Research. Validity: 2019–2028.

Research Interests

Marco is a materials scientist with experience in interdisciplinary projects at the crossroads between physics, chemistry, computer science, mathematics, and data science. He develops predictive modeling techniques based on first principles numerical simulations to help design advanced materials for renewable energy, water, and quantum information technologies.

Quantum simulations First principles and atomistic modeling of materials (solids, liquids, interfaces, nanomaterials): density functional theory, many-body perturbation theory, molecular dynamics, quantum embedding theories.

Molecular engineering Materials for sustainable energy: solar and photoelectrochemical cells, clean water. Materials for quantum information science: quantum computing, quantum sensing, quantum communication, quantum transduction.

Scientific computing Methodology and software development: exascale computing, numerical algorithms, parallel coding, heterogenous computing (GPUs).

Scientific data Artificial intelligence and data science for materials science: property prediction, data repositories, reproducibility of scientific results.

Quantum computing Quantum simulations of materials on noisy intermediate-scale quantum computers.

Invited Presentations

- **Talks as invited speaker**

2024, Aug 27-30 Condensed Matter Theory Annual Meeting, Brixen, Italy. Title: *"Simulating Spin Defects in Solids for Quantum Technologies"*

2024, Jun 10-14 Defect in Solids for Quantum Technologies, Budapest, Hungary. Title: *"Excited State Properties of Point Defects in Solids Investigated with Time-Dependent Density Functional Theory and Quantum Embedding Methods"*

2024, Mag 6-10 Quantum Science Generation, Trento, Italy. Title: *"Simulating condensed systems on quantum computers with quantum embedding"*

2024, Mar 3-8 APS March Meeting 2022: Annual Meeting of the American Physical Society, Minneapolis, MN USA. Title: *"First principles studies of quantum point defects"*

2023, Dec 14-15 High Performance Computing and Quantum Computing – Sixth Edition, CINECA, Casalecchio di Reno, Italy. Title: *"Simulating condensed systems on quantum computers with quantum embedding"*

2023, Jul 18-19 Quantum Computing User Forum, Oak Ridge National Lab, TN USA. Title: *"Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers"*

2023, Jun 13-16 35th Workshop on Recent Developments in Electronic Structure Methods, UC Merced, CA USA. Title: *"First principles studies of quantum point defects"*

2022, Oct 2-5 Co-Design for HPC in Computational Materials and Molecular Science, CECAM, Lausanne Switzerland. Title: *"First principles spectroscopy using pre-exascale and noisy intermediate-scale quantum computers"*

2022, Mar 28-Apr 1 Workshop on Multiscale Approaches in Quantum Mechanics, organized by the Institute for Pure and Applied Mathematics (IPAM), Los Angeles, CA USA. Title: *"Code interoperability extends the scope of first principles spectroscopy"*

2022, Mar 14-18 APS March Meeting 2022: Annual Meeting of the American Physical Society, Chicago, IL USA. Title: *"First principles simulation of neutral excitations in materials"*

2021, Aug 22-26 ACS Fall Meeting, Atlanta, GA USA (virtual). Title: *"First principles simulation of optically activated processes in materials and molecules"*

2020, Jun 7-9 *GW-XL*, GW goes Large Scale, Aalto University, Helsinki, Finland (virtual). Title: *"Large-scale Many-Body Perturbation Theory Calculations"*

2019, May 21-24 Tutorial on writing reproducible workflows for computational materials science, EPFL, Lausanne, Switzerland. Title: *"Qresp, a tool for curating, discovering and exploring reproducible scientific papers"*

2018, Jun 11-15 Materials Genome Initiative at Exascale, Spetses, Greece. Title: *"Coupling first principles molecular with advanced sampling and many body perturbation theory codes"*

2018, Mar 5-9 APS March Meeting 2018: Annual Meeting of the American Physical Society, Los Angeles, CA USA. Title: *"Large-scale first principles calculations with leadership class HPC using many-body perturbation theory"*

2018, Jan 17 High Performance Computing for Manufacturing, Argonne National Lab, IL USA. Title: *"Multiscale modeling of materials interfaces at MICCoM and development of WEST"*

2017, May 30-31 Electrochemical Society Meeting, New Orleans, LA USA. Title: *"Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation, and Applications"*

2017, Feb 27-Mar 3 SIAM Conference on Computer Science and Engineering, Atlanta, GA USA. Title: *"Methodological Developments in the Calculation of Excited-State Properties: Large Scale GW Calculations"*

2017, Jan 12-14 18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, Italy. Title: *"Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation and Applications"*

2016, Oct 24-28 OPTIMADE Workshop: Open Databases Integration for Materials Design, Lorentz Center, Leiden, Netherlands. Title: *"Midwest Integrated Center for Computational Materials (MICCoM): Software, Validation & Data"*

2016, Aug 1-5 TSRC Workshop: Recent Progress in Numerical Green's Functions Methods in Physics and Chemistry, Telluride, CO USA. Title: *"Large scale GW calculations: methodological developments in the computation of excited-state properties"*

2016, Mar 14-18 APS March Meeting 2016: Annual Meeting of the American Physical Society, Baltimore, MD USA. Title: *"Materials by design: methodological developments in the calculation of excited-state properties"*

2016, Jan 18-21 QuantumESPRESSO developers meeting, ICTP, Trieste, Italy. Title: *"WEST: open source software for accurate electronic structure simulations"*

2015, Sept 28-Oct 2 The Intel Xeon Phi User's Group (IXPUG) Annual Meeting, Berkeley, CA USA. Title: *"WEST: Scalable Software for Excited State Properties of Materials and Molecules"*

2014, Aug 10-14 248th ACS National Meeting & Exposition, San Francisco, CA USA. Title: *"Photoexcitations in semiconductors and insulators from first principles"*

- **Seminars as invited speaker**

2023, Sep 18 Seminar, University of Padova, Padova, Italy. Title: *"Quantum embedding methods to simulate condensed systems on quantum computers"*

2023, Apr 14 Condensed Matter Seminar, University of Torino, Torino, Italy. Title: *"First-principles Studies of Quantum Point Defects"*

2023, Jan 17 Molecular foundry distinguished seminar series, Lawrence Berkeley National Laboratory, Berkeley, CA USA. (virtual). Title: *"First-principles Studies of Quantum Point Defects"*

2022, Sep 26 Seminar series on quantum information science, Ames National Laboratory, Ames, IA USA. (virtual). Title: *"First principles spectroscopy using pre-exascale and noisy intermediate-scale quantum computers"*

2021, Nov 8 Condensed matter series seminar, Department of Physics, Case Western Reserve University, Cleveland, OH USA. (virtual). Title: *"First principles simulation of optically activated processes in materials"*

2021, Sep 13 Physics colloquium, Department of Physics, University of Missouri-Columbia, MO USA. (virtual). Title: *"First principles simulation of optically activated processes in materials"*

2020, Aug 5 Intel seminar (virtual). Title: *"Containers enabling interoperable environments in HPC"*

2020, Jul 29 Chicago Quantum Exchange briefing seminar (virtual). Title: *"Quantum simulations of materials on near-term quantum computers"*

2017, Dec 21 Seminar, Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia, Modena, Italy. Title: *"Large Scale Many-Body Perturbation Theory Calculations: Software, Data and Applications"*

2017, Oct 19 Seminar, Department of Physics, Central Michigan University, Mt. Pleasant, MI USA. Title: *"Large Scale Many-Body Perturbation Theory Calculations: Software, Data and Applications"*

Contributed Presentations

2024, Jul 22-25 *Progress in Ensemble Density Functional Theory: Opportunities and Challenges*, Durham, UK. **Talk** "Exploration of the Optical Properties of Point Defects in Semiconductors using TDDFT and Quantum Embedding Methods"

2024, Jul 7-12 *XXXV IUPAP Conference on Computational Physics (CCP2024)*, Thessaloniki, Greece. **Talk** "Exploration of the Optical Properties of Point Defects in Semiconductors and Insulators using Time-dependent Density Functional Theory"

2023, Mar 6-10 *APS March Meeting 2023*, Annual Meeting of the American Physical Society, Las Vegas, NV USA. **Talk** "Green's function formulation of quantum defect embedding theory"

2022, Jun 27-28 *Materials Genome Initiative PI meeting*, College Park, MD USA. **Poster** "Midwest Integrated Center for Computational Materials"

2021, Sept 23-24 *Integrating Quantum Computers in Condensed Matter Physics Simulations*, National Physical Laboratory, London UK (virtual). **Talk** "Quantum simulations of spin-defects in semiconductors"

2021, Mar 15-19 *APS March Meeting 2021*, Annual Meeting of the American Physical Society, Nashville, TN USA (virtual). **Talk** "Quantum simulations of materials on near-term quantum computers", **Talk** "Coupling interoperable software for quantum simulations of materials"

2019, Mar 31-Apr 4 *ACS 2019*, Annual Meeting of the American Chemical Society, Orlando, FL USA. **Talk** "Multisite computations of electronic properties using many-body perturbation theory and interoperable software building blocks"

2019, Mar 4-8 *APS March Meeting 2019*, Annual Meeting of the American Physical Society, Boston, MA USA. **Talk** "Large scale GW and BSE calculations using interoperable software building blocks"

2018, Mar 5-9 *APS March Meeting 2018*, Annual Meeting of the American Physical Society, Los Angeles, CA USA. **Talk** "Raising the bar for accessibility and sustainability of data published in scientific papers"

2017, Mar 13-17 *APS March Meeting 2017*, Annual Meeting of the American Physical Society, New Orleans, LA USA. **Talk** "Large Scale Many-Body Perturbation Theory calculations: methodological developments, data collections, validation"

2016, Jun 1-5 *LUEST 2016*, Low-scaling and Unconventional Electronic Structure Techniques Conference, Telluride, CO USA. **Poster** "Computing quasiparticle energies for large systems Without Empty STates (WEST)"

2016, May 2-3 *CHiMaD Workshop*, CHiMaD Data, Databases & Discovery Workshop, Evanston, IL USA. **Talk** "Midwest Integrated Center for Computational Materials (MICCoM)

2015, Dec 18 Physics in Modena 2015, Annual meeting of the University of Modena and Reggio Emilia alumni, Modena, Italy. Title: *"From punched cards to modern HPC supercomputers: electronic structure methods"*

2015, Apr 8-10 *2015 Mach Conference*, Multiscale research in materials, Annapolis, MD USA. **Talk** "High performance electronic structure engineering"

2015, Mar 2-6 *APS March Meeting 2015*, Annual Meeting of the American Physical Society, San Antonio, TX USA. **Talk** "High performance electronic structure engineering"

2015, Jan 15-17 *Total Energy 2015*, International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, Italy. **Poster** "High performance electronic structure engineering with hybrid DFT and GW"

2015, Jan 14 *QE 2015*, QuantumESPRESSO developers meeting, ICTP, Trieste, Italy. **Talk** "New developments in GW and in hybrid functionals"

2014, Mar 3-7 *APS March Meeting 2014*, Annual Meeting of the American Physical Society, Denver, CO USA. **Talk** "Computing quasiparticle energies and band offsets for large systems"

2013, Jul 11-16 *Gordon Research Conference*, Time-dependent Density-functional Theory, University of New England, Biddeford, ME USA. **Poster** "Computing quasiparticle energies for large systems"

2013, Mar 18-22 *APS March Meeting 2013*, Annual Meeting of the American Physical Society, Baltimore, MD USA. **Talk** "Computational spectroscopy of nanocomposites"

2012, Sep 17-21 *EMRS Fall Meeting 2012*, Conference of the European Materials Research Society, Warsaw, Poland. **Talk** "Carrier Multiplication in isolated and interacting silicon nanocrystals for photovoltaic applications by ab initio calculations"

2012, Sep 10-14 *CECAM conference*, Energy from the Sun: Computational Chemists and Physicists Take up the Challenge, Chia (CA), Italy. **Poster** "Is Nanocrystal Interaction Useful for Photovoltaic Applications?"

2011, Sep 27-30 *ETSF-2011*, 16^{th} ETSF Workshop on Electronic Excitations, Turin, Italy. **Talk** "Auger Recombination and Impact Ionization from first-principles: from bulk to nanocrystals"

2011, May 16-20 *YRM11*, 8^{th} Nanoquanta-ETSF Young Researchers Meeting, Physics Dept. of the University Federico II, Naples, Italy. **Talk** "Auger Recombination in Si and GaAs from first-principles"

2011, Feb 21-22 *DMD-TeoC*, First Italian Workshop on Computational Nanoscience, CNR, Rome, Italy. **Poster** "Auger Recombination in Si and GaAs semiconductors: ab initio results"

2010, Jan 02-15 *Time-Dependent Density-Functional Theory: Prospects and Applications*, 4th International Workshop and School, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain. **Poster** "Ab-initio calculation of the Impact Ionization Rate in GaAs using Yambo code"

2009, Sep 27-29 *New Frontiers in Casimir Force Control*, Satellite workshop of QFEXT09 conference, Santa Fe, NM USA. **Poster** "First principle calculations of the Casimir force between Silicon films", **Poster** "Role and applications of the vacuum force in microscopic systems"

2009, Sep 21-25 *QFEXT09*, 9^{th} conference on Quantum Field Theory Under The Influence of External Conditions, devoted to the Centenary of H. B. G. Casimir, The University of Oklahoma, Norman, OK USA. **Talk** "First principle calculations of the Casimir force between Silicon films"

2009, Jun 10-11 *HERODOT09*, Workshop on Theory and Modeling of Quantum Confined Materials, ISEN, Lille, France. **Poster** "A simple ab-initio calculation of the optical gain in Si-nc"

2009, Jun 2-6 *YRM09*, 6^{th} Nanoquanta-ETSF Young Researchers Meeting, Theoretical Physics Dept. of the Free University Berlin, Germany. **Poster** "A simple ab-initio calculation of the optical gain in Si-nc"

Publications

IDs

Google Scholar ID: *Hi6sN5EAAAAJ*

Scopus Author ID: *56346821300*

ResearcherID: *AAT-1971-2020*

ORCID: *0000-0001-6303-2403*

Preprints

3. *Many-body perturbation theory with hybrid density functional theory starting points accelerated by adaptively compressed exchange*, V. W-z. Yu, M. Govoni, **arXiv** (2024). arXiv:2409.14662.
2. *Photoactivation of color centers induced by laser irradiation in ion-implanted diamond*, V. Pugliese, E. Nieto Hernández, E. Corte, M. Govoni, S. Ditalia Tchernij, P. Olivero, J. Forneris, **arXiv** (2024). arXiv:2409.06359.
1. *GPU-Accelerated Solution of the Bethe-Salpeter Equation for Large and Heterogeneous Systems*, V. W-z. Yu, Y. Jin, G. Galli, M. Govoni, **arXiv** (2024). arXiv:2409.15116.

Articles

50. *Self-Trapped Excitons in Metal-Halide Perovskites Investigated by Time-Dependent Density Functional Theory*, Y. Jin, M. Rusishvili, M. Govoni, G. Galli, **J. Phys. Chem. Lett.** 15, 3229 (2024). DOI:10.1021/acs.jpclett.4c00209.
49. *Excited State Properties of Point Defects in Semiconductors and Insulators Investigated with Time-Dependent Density Functional Theory*, Y. Jin, V. W. Yu, M. Govoni, A.C. Xu, and G. Galli, **J. Chem. Theory Comput.** 19, 8689 (2023). DOI:10.1021/acs.jctc.3c00986.
48. *Nonempirical Range-Separated Hybrid Functional with Spatially Dependent Screened Exchange*, J. Zhan, M. Govoni, G. Galli, **J. Chem. Theory Comput.** 19, 5851 (2023). DOI:10.1021/acs.jctc.3c00580.
47. *Roadmap on Electronic Structure Codes in the Exascale Era*, V. Gavini, S. Baroni, V. Blum, D.R. Bowler, A. Buccheri, J.R. Chelikowsky, S. Das, W. Dawson, P. Delugas, M. Dogan, C. Draxl, G. Galli, L. Genovese, P. Giannozzi, M. Giantomassi, X. Gonze, M. Govoni, A. Gulans, F. Gygi, J.M. Herbert, S. Kokott, T.D. Kühne, K.-H. Liou, T. Miyazaki, P. Motamarri, A. Nakata, J.E. Pask, C. Plessl, L.E. Ratcliff, R.M. Richard, M. Rossi, R. Schade, M. Scheffler, O. Schütt, P. Suryanarayana, M. Torrent, L. Truflandier, T.L. Windus, Q. Xu, V.W.-Z. Yu, D. Perez, **Modelling Simul. Mater. Sci. Eng.** 31, 063301 (2023), DOI:10.1088/1361-651X/acdf06.
46. *Quantum simulations of Fermionic Hamiltonians with efficient encoding and ansatz schemes*, B. Huang, N. Sheng, M. Govoni, G. Galli, **J. Chem. Theory Comput.** 19, 1487 (2023), DOI:10.1021/acs.jctc.2c01119.
45. *Vibrationally resolved optical excitations of the nitrogen-vacancy center in diamond*, Y. Jin, M. Govoni, and G. Galli, **npj Comput. Mater.** 8, 238 (2022), DOI:10.1038/s41524-022-00928-y.
44. *Computational protocol to evaluate electron-phonon interactions within density matrix perturbation theory*, H. Yang, M. Govoni, A. Kundu, and G. Galli, **J. Chem. Theory Comput.** 18, 6031 (2022), DOI:10.1021/acs.jctc.2c00579.

43. *GPU Acceleration of Large-Scale Full-Frequency GW Calculations*, W. Yu, and M. Govoni, **J. Chem. Theory Comput.** 18, 4690 (2022), DOI:10.1021/acs.jctc.2c00241.

42. *Quantum Embedding Theories to Simulate Condensed Systems on Quantum Computers*, N. Sheng, C. Vorwerk, B. Huang, M. Govoni, and G. Galli, **Nature Comput. Sci.** 2, 424 (2022), DOI:10.1038/s43588-022-00279-0.

41. *Green's function formulation of quantum defect embedding theory*, N. Sheng, C. Vorwerk, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 18, 3512 (2022), DOI: 10.1021/acs.jctc.2c00240

40. *Simulating the electronic structure of spin defects on quantum computers*, B. Huang, M. Govoni, and G. Galli, **PRX Quantum** 3, 010339 (2022), DOI: 10.1103/PRXQuantum.3.010339

39. *Combined first-principles calculations of electron-electron and electron-phonon self-energies in condensed systems*, H. Yang, M. Govoni, A. Kundu, and G. Galli, **J. Chem. Theory Comput.** 17, 7468 (2021), DOI: 10.1021/acs.jctc.1c00605

38. *Photoluminescence spectra of point defects in semiconductors: validation of first principles calculations*, Y. Jin, M. Govoni, G. Wolfowicz, S.E. Sullivan, F.J. Heremans, D.D. Awschalom, and G. Galli, **Phys. Rev. Mater.** 5, 084603 (2021), DOI: 10.1103/PhysRevMaterials.5.084603

37. *Quantum vibronic effects on the electronic properties of solid and molecular carbon*, A. Kundu, M. Govoni, H. Yang, M. Ceriotti, F. Gygi, and G. Galli, **Phys. Rev. Mater.** 5, L070801 (2021), DOI: 10.1103/PhysRevMaterials.5.L070801

36. *OPTIMADE: an API for exchanging materials data*, C.W. Andersen, R. Armiento, E. Blokhin, G.J. Conduit, S. Dwaraknath, M.L. Evans, Á. Fekete, A. Gopakumar, S. Gražulis, A. Merkys, F. Mohamed, C. Oses, G. Pizzi, G. Rignanese, M. Scheidgen, L. Talirz, C. Toher, D. Winston, R. Aversa, K. Choudhary, P. Colinet, S. Curtarolo, D. Di Stefano, C. Draxl, S. Er, M. Esters, M. Fornari, M. Giantomassi, M. Govoni, G. Hautier, V. Hegde, M.K. Horton, P. Huck, G. Huhs, J. Hummelshøj, A. Kariryaa, B. Kozinsky, S. Kumbhar, M. Liu, N. Marzari, A.J. Morris, A. Mostofi, K.A. Persson, G. Petretto, T. Purcell, F. Ricci, F. Rose, M. Scheffler, D. Speckhard, M. Uhrin, A. Vaitkus, P. Villars, D. Waroquiers, C. Wolverton, M. Wu, and X. Yang, **Sci. Data** 8, 217 (2021), DOI:10.1038/s41597-021-00974-z

35. *Quantum Embedding Theory for Strongly-correlated States in Materials*, H. Ma, N. Sheng, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 17, 2116 (2021), DOI: 10.1021/acs.jctc.0c01258

34. *Machine Learning Dielectric Screening for the Simulation of Excited State Properties of Molecules and Materials*, S. Dong, M. Govoni, and G. Galli, **Chem. Sci.** 12, 4970 (2021), DOI: 10.1039/D1SC00503K

33. *Code interoperability extends the scope of quantum simulations*, M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, and G. Galli, **npj Comput. Mater.** 7, 32 (2021), DOI: 10.1038/s41524-021-00501-z

32. *First-principles Studies of Strongly Correlated States in Defect Spin Qubits in Diamond*, H. Ma, N. Sheng, M. Govoni, and G. Galli, **Phys. Chem. Chem. Phys.** 22, 25522 (2020), DOI: 10.1039/D0CP04585C

31. *Quantum simulations of materials on near-term quantum computers*, H. Ma, M. Govoni, and G. Galli, **npj Comput. Mater.** 6, 85 (2020), DOI: 10.1038/s41524-020-00353-z

30. *PyCDFT: A Python package for constrained density functional theory*, H. Ma, W. Wang, S. Kim, M.-H. Cheng, M. Govoni, and G. Galli, **J. Comp. Chem.** 41, 1859 (2020), DOI: 10.1002/jcc.26354

29. *PyZFS: A Python package for first-principles calculations of zero-field splitting tensors*, H. Ma, M. Govoni, and G. Galli, **J. Open Source Softw.** 5(47), 2160 (2020), DOI: 10.21105/joss.02160

28. *MatD^3: A Database and Online Presentation Package for Research Data Supporting Materials Discovery, Design, and Dissemination*, R. Laasner, X. Du, A. Tanikanti, C. Clayton, M. Govoni, G. Galli, M. Ropo, and V. Blum, **J. Open Source Softw.** 5(45), 1945 (2020), DOI: 10.21105/joss.01945

27. *Improving the efficiency of G_0W_0 calculations with approximate spectral decompositions of dielectric matrices*, H. Yang, M. Govoni, and G. Galli, **J. Chem. Phys.** 151, 224102 (2019), DOI: 10.1063/1.5126214

26. *Finite field approach to solving the Bethe Salpeter equation*, N. L. Nguyen, H. Ma, M. Govoni, F. Gygi, and G. Galli, **Phys. Rev. Lett.** 122, 237402 (2019), DOI: 10.1103/PhysRevLett.122.237402

25. *Dielectric dependent hybrid functionals for heterogeneous materials*, H. Zheng, M. Govoni, and G. Galli, **Phys. Rev. Mater.** 3, 073803 (2019), DOI: 10.1103/PhysRevMaterials.3.073803

24. *Qresp, a tool for curating, discovering and exploring reproducible scientific papers*, M. Govoni, M. Munakami, A. Tanikanti, J. Skone, H. Runesha, F. Giberti, J. de Pablo, and G. Galli, **Sci. Data** 6, 190002 (2019), DOI: 10.1038/sdata.2019.2

23. *A Finite-field Approach for GW Calculations Beyond the Random Phase Approximation*, H. Ma, M. Govoni, F. Gygi, and G. Galli, **J. Chem. Theory Comput.** 15, 154 (2019), DOI: 10.1021/acs.jctc.8b00864

22. *The role of defects and excess surface charges at finite temperature for optimizing oxide photoabsorbers*, M. Gerosa, F. Gygi, M. Govoni, and G. Galli, **Nature Materials** 17, 1122 (2018), DOI: 10.1038/s41563-018-0192-4

21. *Fundamental Principles for Calculating Charged Defect Ionization Energies in Ultrathin Two-Dimensional Materials*, T.J. Smart, F. Wu, M. Govoni, and Y. Ping, **Phys. Rev. Mater.** 2, 124002 (2018), DOI: 10.1103/PhysRevMaterials.2.124002

20. *Coupling First-Principles Calculations of Electron-Electron and Electron-Phonon Scattering, and Applications to Carbon-Based Nanostructures*, R. McAvoy, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 14, 6269 (2018), DOI: 10.1021/acs.jctc.8b00728

19. *Dielectric properties of condensed systems composed of fragments*, D. Pan, M. Govoni, and G. Galli, **J. Chem. Phys.** 149, 051101 (2018), DOI: 10.1063/1.5044636
18. *GW100: Comparison of Methods and Accuracy of Results Obtained with the WEST Code*, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 14, 1895 (2018), DOI: 10.1021/acs.jctc.7b00952
17. *Electron affinity of liquid water*, A. Gaiduk, T.A. Pham, M. Govoni, F. Paesani, and G. Galli, **Nature Comm.** 9, 247 (2018), DOI: 10.1038/s41467-017-02673-z
16. *Designing defect-based qubit candidates in wide-gap binary semiconductors for solid-state quantum technologies*, H. Seo, H. Ma, M. Govoni, and G. Galli, **Phys. Rev. Mater.** 14, 1700198 (2017), DOI: 10.1103/PhysRevMaterials.1.075002
15. *Carrier Multiplication in Silicon Nanocrystals: Theoretical Methodologies and Role of the Passivation*, I. Marri, M. Govoni, and S. Ossicini, **Phys. Status Solidi C** 1, 075002 (2017), DOI: 10.1002/pssc.201700198
14. *Performance and self-consistency of the generalized dielectric dependent hybrid functional*, N. Brawand, M. Govoni, M. Vörös, and G. Galli, **J. Chem. Theory Comput.** 13, 3318 (2017), DOI: 10.1021/acs.jctc.7b00368
13. *Electronic Structure of Aqueous Solutions: Bridging the Gap Between Theory and Experiments*, T.A. Pham, M. Govoni, R. Seidel, S.E. Bradforth, E. Schwegler, and G. Galli, **Science Advances** 3 (6), 1603210 (2017), DOI: 10.1126/sciadv.1603210
12. *Generalization of dielectric dependent hybrid functionals to finite systems*, N. Brawand, M. Vörös, M. Govoni, and G. Galli, **Phys. Rev. X** 6, 041002 (2016), DOI: 10.1103/PhysRevX.6.041002
11. *Implementation and Validation of Fully-Relativistic GW Calculations: Spin-Orbit Coupling in Molecules, Nanocrystals and Solids*, P. Scherpelz, M. Govoni, I. Hamada, and G. Galli, **J. Chem. Theory Comput.** 12, 3523 (2016), DOI: 10.1021/acs.jctc.6b00114
10. *Nonempirical range-separated hybrid functionals for solids and molecules*, J. Skone, M. Govoni, and G. Galli, **Phys. Rev. B** 93, 235106 (2016), DOI: 10.1103/PhysRevB.93.235106
9. *Photoelectron spectra of aqueous solutions from first principles*, A. P. Gaiduk, M. Govoni, R. Seidel, J. Skone, B. Winter, and G. Galli, **J. Am. Chem. Soc. Commun.** 138, 6912 (2016), DOI: 10.1021/jacs.6b00225
8. *Design of defect spins in piezoelectric aluminum nitride for solid-state hybrid quantum technologies*, H. Seo, M. Govoni, and G. Galli, **Scientific Reports** 6, 20803 (2016), DOI: 10.1038/srep20803
7. *First-principles calculations of electronic coupling effects in silicon nanocrystals: Influence on near band-edge states and on carrier multiplication processes*, I. Marri, M. Govoni, and S. Ossicini, **Sol. Energ. Mat. Sol. C.** 145, 162 (2016), DOI: 10.1016/j.solmat.2015.07.013
6. *Large scale GW calculations*, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 11, 2680 (2015), DOI: 10.1021/ct500958p

5. *Carrier multiplication in silicon nanocrystals: ab-initio results*, I. Marri, M. Govoni, and S. Ossicini, **Beilstein J. Nanotechnol.** 6, 343 (2015), DOI: 10.3762/bjnano.6.33
4. *Red-shifted carrier multiplication energy threshold and exciton recycling mechanisms in strongly interacting silicon nanocrystals*, I. Marri, M. Govoni, and S. Ossicini, **J. Am. Chem. Soc.** 136, 13257 (2014), DOI: 10.1021/ja5057328
3. *Self-consistent hybrid functional for condensed systems*, J.H. Skone, M. Govoni, and G. Galli, **Phys. Rev. B** 89, 195112 (2014), DOI: 10.1103/PhysRevB.89.195112
2. *Carrier multiplication between interacting nanocrystals for fostering silicon-based photovoltaics*, M. Govoni, I. Marri, and S. Ossicini, **Nature Photonics** 6, 672–679 (2012), DOI: 10.1038/nphoton.2012.206
1. *Auger Recombination in Si and GaAs semiconductors: Ab initio results*, M. Govoni, I. Marri, and S. Ossicini, **Phys. Rev. B** 84, 075215 (2011), DOI: 10.1103/PhysRevB.84.075215

Technical reports

1. *First-Principles Simulations of Functional Materials for Energy Conversion*, H. Zheng, C. Knight, M. Govoni, G. Galli, and F. Gygi, Technical Report for the ALCF Theta Early Science Program (2017), DOI: 10.2172/1490828

Book chapters

1. *Carrier Multiplication in Isolated and Interacting Silicon Nanocrystals*, I. Marri, M. Govoni, and S. Ossicini, Nanotechnology and Photovoltaic Devices: Light Energy Harvesting with Group IV Nanostructures. 177 -202; Editors: J. Valenta and S. Mirabella (2015), DOI: 10.1201/b18090-7

Proceedings

1. *Role of surface states in the Casimir force between semiconducting films*, M. Govoni, A. Benassi, and C. Calandra, Proceedings of the Ninth Conference on Quantum Field Theory under the Influence of External Conditions (QFEXT09), Editors: KA. Milton, M. Bordag, World Scientific (2009), DOI: 10.1142/9789814289931_0031

Research support

- **Current support:**

2024 – 2029 FIS Starting Grant, "*Designing Solid-State Spin Qubits*", Research Project funded by the Italian Ministry of University and Research (ERC Panel: PE3 – Condensed Matter Physics); PI: M. Govoni (Unimore), Total Award: €778,656 for 5 years.

2023 – 2025 PRIN PNRR 2022, "*Opto-mechanical effects in spin-defects for quantum technologies*", Research Project of National Interest funded by the Italian Ministry of University and Research; PI: M. Govoni (Unimore), co-PIs: J. Forneris (Unito), Total Award: €231,259 for 2 years. (€149,000 to Unimore)

2023 – 2026 DOE/BES, "*Midwest Integrated Center for Computational Materials*" (*MICCoM-3*), Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences; PI: G. Galli (ANL/UChicago), co-PIs: M. Govoni (Unimore), M. Chan (ANL), J. Heremans (ANL), F. Gygi (UCDavis), J. Whitmer (UNotreDame), D. Talapin (UChicago), A. Ferguson (UChicago), J. de Pablo (ANL/UChicago), J. Xu (ANL), Total Award: \$3,000,000/year. (€500,000 to Unimore, http://miccom-center.org)

2024 – 2025 Cascade Grant of the National Quantum Science & Technology Institute (NQSTI), "*Emergent topological states in semiconductor-ferromagnet van der Waals heterostructures*", Research Project funded by the Italian Ministry of University and Research; PI: M. Gibertini (Unimore), co-PI: M. Govoni (Unimore), Total Award: €233,624 for 2 years.

- **Completed support:**

2020 – 2023 DOE/BES, "*Optical Control of Spin-polarization in Quantum Materials*", U.S. Department of Energy, Early Career Research Program (ECRP); PI: M. Govoni (ANL), Total Award: \$500,000/year. (https://science.osti.gov/early-career)

2019 – 2023 DOE/BES, "*Midwest Integrated Center for Computational Materials*" (*MICCoM-2*), Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences; PI: G. Galli (ANL/UChicago), co-PIs: M. Govoni (ANL/Unimore), M. Chan (ANL), J. Heremans (ANL), F. Gygi (UCDavis), J. Whitmer (UNotreDame), D. Talapin (UChicago), A. Ferguson (UChicago), J. de Pablo (ANL/UChicago), Total Award: \$2,500,000/year. (http://miccom-center.org)

2021 – 2023 DOE/BES, "*The Atomic Quantum Information Surface Science (AQuISS) Lab*", Quantum Information Science and Research Infrastructure program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences; PI: J. Guest (ANL), co-PIs: M. Govoni (ANL), M. Chan (ANL), P. Darancet (ANL), D. Gosztola (ANL), N. Guisinger (ANL), A. High (UChicago), X. Ma (ANL), D. Rosenmann (ANL), Total Award: \$1,000,000/year.

2021 – 2023 ANL-LDRD, "*Broadband Directional Detection of Electromagnetic Pulses Using Quantum Sensing*"; PI: A. Yanguas-Gil (ANL), co-PIs: M. Govoni (ANL), J. Heremas (ANL). Total Award: \$260,000/year.

2019 – 2022 NERSC-NESAP, "*Many-Body Perturbation Theory with WEST*", NERSC Exascale Science Application Program (NESAP) Tier 1 research project; PI: M. Govoni (ANL), Total Award: 1 assigned postdoctoral researcher at U.S. National Energy Research Scientific Computing (NERSC).

2019 ANL-LDRD, "*Benchmark and Optimization of 3D-FFT Solvers for Many-Body Perturbation Theory Calculations*"; PI: M. Govoni (ANL), Total Award: \$32,000.

2018 ANL-LDRD, "*For Everyone A21: Distributed Electronic Structure Calculations Using A Globus-enabled Programmable Cyberinfrastructure*"; PI: M. Govoni (ANL), Total Award: \$25,000.

2015 – 2019 DOE/BES, "*Midwest Integrated Center for Computational Materials*" (*MICCoM-1*), Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences; PI: G. Galli (ANL/UChicago), co-PIs: M. Govoni (ANL), M. Chan (ANL), O. Heinonen (ANL), N. Ferrier (ANL), J. Mitchell (ANL), S. Glotzer (UMichigan), F. Gygi (UCDavis), J. Whitmer (UNotreDame), D. Talapin (UChicago), M. Kanatzidis (ANL/Northwestern), M. Olvera de la Cruz (Northwestern), J. de Pablo (ANL/UChicago), Total Award: $3,000,000/year. (http://miccom-center.org)

2016 – 2018 *ESP*, "*Early Science Program Theta*", Research grant to get early access to the ANL-ALCF Theta machine; PI: G. Galli (ANL/UChicago), co-PIs: M. Govoni (ANL), F. Gygi (UCDavis). Total Award: 1 fully funded postdoc and computational resources at ANL-ALCF.

2010 – 2011 HPC-EUROPA2, "*Ab initio calculations of out-of-equilibrium quasiparticle self-energies applied to highly excited Silicon Nanocrystals*", HPC research grant: HPC-EUROPA2; PI: M. Govoni (Unimore), Total Award: 6 Weeks of paid short-term visit to Institute Néel, Grenoble, France.

(Note: PI identifies the Principal Investigator)

Computational Projects

2023 Euro-HPC Extreme scale, "*Designing point-defects in low-dimensional materials with quantum characteristics*", funded by the Euro-HPC Joint Undertaking; PI: M. Govoni (Unimore), Total Award: 21,602,304 core hours on CINECA/LeonardoBOOSTER.

2023 ISCRA-B, "*First-principles simulations of point-defects in 2D Moiré lattices*", funded by the ISCRA Consortium; PI: M. Govoni (Unimore), Total Award: 135,168 GPU hours on CINECA/LeonardoBOOSTER.

2022 Award to use dedicated IBM Q resources (quantum computers) to develop hybrid classical-quantum electronic structure simulations, funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: Premium access to IBM Q Hub.

2022 ALCC, "*First principles simulations of correlated quantum matter*", ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: 135,168 node-hours on OLCF/Summit, 25,000 node-hours on ALCF/Theta, 160,000 node-hours on NERSC/Cori.

2022 NERSC award, "*Quantum Computing for Materials Science: Simulation of Defects in Materials for Quantum Information Science*", NERSC award dedicated to projects on Quantum Information Science, funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: 25,000 GPU node hours on NERSC/Perlmutter.

2022 INCITE, "*Large-Scale Simulations of Light-Activated Matter*", Innovative and Novel Computational Impact on Theory and Experiment (INCITE), funded by the US Department of Energy; PI: G. Galli (UChicago/ANL), co-PIs: M. Govoni (ANL), F. Gygi (UCDavis), Total Award: 600,000 node hours on ANL/Theta; 290,000 node hours on ORNL/Summit.

2021 OLCF Director's Discretionary allocation; PI: M. Govoni (ANL), Total Award: 20,000 node hours on ORNL/Summit.

2021 Award to use dedicated IBM Q resources (quantum computers) to develop hybrid classical-quantum electronic structure simulations, funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: Premium access to IBM Q Hub.

2021 OLCF Director's Discretionary allocation; PI: M. Govoni (ANL), Total Award: 15,000 node hours on ORNL/Summit.

2021 INCITE, "*Large-Scale Simulations of Light-Activated Matter*", Innovative and Novel Computational Impact on Theory and Experiment (INCITE), funded by the US Department of Energy; PI: G. Galli (UChicago/ANL), co-PIs: M. Govoni (ANL), F. Gygi (UCDavis), Total Award: 1,200,000 node hours on ANL/Theta.

2020 ALCC, "*Benchmarking Many-Body Perturbation Theory*", ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy; PI: O. Heinonen (ANL), co-PIs: M. Govoni (ANL), A. Benali (ANL), Total Award: 100,000 node hours on ANL/Theta.

2019 ADSP, "*Advanced Materials Characterization with AI-Informed Computation*", Argonne Data Science Program (ADSP); PI: M. Govoni (ANL), co-PI: S. Dong (ANL), Total Award: two assigned staff scientists at Argonne National Leadership Computing Facility (ALCF) and 4,000,000 core hours.

2017 ALCC, "*Computational engineering of electron-vibration coupling mechanisms*", ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy; PI: M. Govoni (ANL). Total Award: 60,000,000 core hours.

2017 NERSC-ERCAP, "*GW for the materials science community: extending transferability, benchmarking and addition of new productivity tools within the WEST code*"; PI: M. Govoni (ANL), co-PI: J. Skone (UChicago), Total Award: 3,000,000 core hours.

2016 ALCC, "*Computational engineering of defects in soft and hard materials for energy and quantum information applications*", ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: 53,700,000 core hours.

2016 NERSC-ERCAP, "*GW for the materials science community: extending transferability, benchmarking and addition of new productivity tools within the WEST code*"; PI: M. Govoni (ANL), co-PI: J. Skone (UChicago), Total Award: 3,000,000 core hours.

2016 NERSC-ERCAP, "*Structure and stability of solids of nanoparticles from first principles*"; PI: M. Handlin (UChicago), co-PI: M. Govoni (ANL), Total Award: 1,000,000 core hours.

2016 NERSC-ERCAP, "*Large scale calculations on nanostructured heterogeneous interfaces*"; PI: M. Vörös (UChicago), co-PI: M. Govoni (ANL), Total Award: 3,000,000 core hours.

2016 ANL-CNM, "*Structure and stability of solids of nanoparticles from first principles*"; PI: M. Govoni (ANL), Total Award: 870,000 core hours.

2016 ANL-LCRC, "*GW for the materials science community*"; PI: M. Govoni (ANL), Total Award: 1,000,000 core hours.

2015 ALCC, "*First principles large scale simulations of interfaces for energy conversion and storage*", ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy; PI: M. Govoni (ANL), Total Award: 75,000,000 core hours (IBM BG/Q Mira).

2015 NERSC-ERCAP, "*Ab-initio Photo-Electro-Chemical study of interfaces for water splitting*", PI: M. Govoni (ANL), Total Award: 2,000,000 core hours.

2015 NERSC-NISE, "*Large scale calculations on nanostructured heterogeneous interfaces*" (Larnint2015); PI: M. Vörös (Uchicago), co-PI: M. Govoni (ANL), Total Award: 2,000,000 core hours.

2014 PRACE, "*Multiple Exciton Generation: Application to PhotoVoltaic*" (MEGAPV); PI: S. Ossicini (Unimore), co-PIs: M. Govoni (UChicago), I. Marri (Unimore), Total Award: 32,000,000 core hours (IBM BG/Q Fermi).

2014 CINECA-ISCRA B, "*simulaTiOn of neW carriER multiplication mechanisms in silicon NanocrYstals*" (TOWER-NY); PI: I. Marri (Unimore), co-PI: M. Govoni (Uchicago), Total Award; 7,800,000 core hours (IBM BG/Q Fermi).

2014 NERSC-NISE, "*Large scale calculations on nanostructured heterogeneous interfaces*" (Larnint2014); PI: M. Vörös (Uchicago), co-PI: M. Govoni (Uchicago), Total Award: 5,000,000 core hours.

2013 CINECA-ISCRA A, "*Multiexcitons at a cOst of one: carrier MultiplicAtion in silicon NanocrYstals*" (MOMA-NY); PI: I. Marri (Unimore), co-PI: M. Govoni (UCDavis), Total Award: 8,000,000 core hours (IBM BG/Q Fermi).

2012 PRACE, "*High perfOrmance compuTing in Silicon nanostructrUres for third generatioN photovoltaics*" (HOTSUN); PI: S. Ossicini (Unimore), co-PIs: M. Govoni (Unimore), I. Marri (Unimore), Total Award: 10,500,000 core hours (IBM BG/Q Fermi).

2011 CINECA-ISCRA B, "*Multiple Exciton Generation in Si nanostrUctures for photovoltaic applicatioNs*" (MEGINSUN); PI: M. Govoni (Unimore), Total Award: 150,000 core hours.

2011 CINECA-ISCRA C, "*Fast-recombination by Surface States in Silicon Nanocrystals*" (FARESSSN); PI: M. Govoni (Unimore), Total Award: 48,000,000 core hours.

2011 CINECA-ISCRA C, "*PHOnon Spectra in SI nanocrystals*" (PHOSSI); PI: M. Govoni (Unimore), Total Award: 20,000 core hours.

2011 CASPUR-Standard, "*Auger Recombination in Silicon Nano-Crystals*"; PI: M. Govoni (Unimore), Total Award: 63,000 core hours.

2010 CINECA-ISCRA C, "*Ab initio Calculations of Out-of-equilibrium quasiparticle SElf energies applied to highly excited Silicon NANOcrystals*" (COSENANO); PI: M. Govoni (Unimore), Total Award: 20,000 core hours.

2010 CINECA-ISCRA C, "*Carrier Multiplication in Si-nanostructures*" (CAMUSI); PI: M. Govoni (Unimore), Total Award: 20,000 core hours.

Teaching

- **PhD courses**

2023/2024 *Applied Quantum Computing to Atomistic Simulations of Molecules and Materials*, PhD in Physics and Nanosciences, University of Modena and Reggio Emilia.

- **Master courses**

2023–2024 *Theory and Simulation of Excitations in Materials*, M.Sc in Physics, University of Modena and Reggio Emilia.

2023–2024 *High Performance Computing for Advanced Physical Analysis*, M.Eng. in Digital Automation Engineering, University of Modena and Reggio Emilia.

2022–2023 *Atomistic Simulation Methods*, M.Sc in Physics, University of Modena and Reggio Emilia.

2022–2023 *Applied Scientific Computing in Molecular Engineering*, M.Sc. in Molecular Engineering, University of Chicago.

2021–2022 *Applied Scientific Computing in Molecular Engineering*, M.Sc. in Molecular Engineering, University of Chicago.

2020–2021 *Applied Scientific Computing in Molecular Engineering*, M.Sc. in Molecular Engineering, University of Chicago.

2019–2020 *Applied Scientific Computing in Molecular Engineering*, M.Sc. in Molecular Engineering, University of Chicago.

- **Bachelor courses**

2024–2025 *Classical Physics*, B.Eng in Computer Science, University of Modena and Reggio Emilia.

- **Schools, Lecture series, workshops**

2023 Instructor. *MICCoM Computational Lecture series*, 2 lectures on quantum many-body physics and computational spectroscopy. Pritzker School of Molecular Engineering, University of Chicago.

2017 Instructor and organizer. *MICCoM Computational School*, Pritzker School of Molecular Engineering, University of Chicago.

- **Teaching assistant**

2011–2012 Teaching Assistant. Undergraduate course *Quantum Mechanics*, held by Prof. Carlo Jacoboni, B.Sc. in Physics, University of Modena and Reggio Emilia.

2010–2011 Teaching Assistant. Undergraduate course *Quantum Mechanics*, held by Prof. Carlo Jacoboni, B.Sc. in Physics, University of Modena and Reggio Emilia.

2009–2010 Teaching Assistant. Undergraduate course *Quantum Mechanics*, held by Prof. Carlo Jacoboni, B.Sc. in Physics, University of Modena and Reggio Emilia.

Supervision

- **Software/data engineers**

2019–2020 Sushant Bansal, University of Chicago
2017–2019 Aditya Tanikanti, University of Chicago

- **Postdoctoral research advisees**

2021–2023 Wenzhe Yu, Argonne National Laboratory
2022–2023 John McFarland, Argonne National Laboratory
2019–2022 Soham Ghosh, NERSC (co-supervised)
2021–2022 Christian Vorwerk, University of Chicago (co-supervised)
2019–2021 Arpan Kundu, University of Chicago (co-supervised)
2020–2021 Lan Huang, Argonne National Laboratory
2018–2020 Sijia Dong, Argonne National Laboratory (co-supervised)
2016–2018 Huihuo Zheng, Argonne National Laboratory (co-supervised)

- **Doctoral research advisees**

2024–present Lorenzo Gottardi, University of Modena and Reggio Emilia
2024–present Pietro Martinello, University of Modena and Reggio Emilia
2023–present Alessandro Bello, University of Modena and Reggio Emilia
2021–2023 Jiawei Zhan, University of Chicago (co-supervised)
2020–2023 Benchen Huang, University of Chicago (co-supervised)
2019–2023 Yu Jin, University of Chicago (co-supervised)
2020–2023 Andrew Xu, University of Chicago (co-supervised)
2022 Matthew Pham, University of Chicago
2020–2022 Nan Sheng, University of Chicago (co-supervised)
2016–2021 Han Yang, University of Chicago (co-supervised)
2016–2020 He Ma, University of Chicago (co-supervised)
2016–2018 Nicholas Brawand, University of Chicago (co-supervised)
2016–2018 Ryan McAvoy, University of Chicago (co-supervised)

- **Undergraduate research advisees**

2019 Mohammed Alsenani, University of Chicago (co-supervised)

Scientific Visits

2016 Nov-Dec National Institute for Materials Science, Tsukuba, Japan, host: Prof. Ikutaro Hamada
2010 Jun-Jul Institute Néel, Grenoble, France, host: Dr. Claudio Attaccalite

Professional Service

- **Institutional**

2023–present Board Member of the Graduate School, PhD School in Physics and Nanoscience, University of Modena and Reggio Emilia.

2023 Organized the event "La Ricerca in FISICA", a crosscutting event for students of both the Bachelor and Master degrees in Physics at Unimore. The event was designed to engage students by presenting the research activities in physics at Unimore while simulating a conference setting, i.e., with keynotes followed by a poster session.

2021 Organized the Argonne's Materials Science Division retreat on AI and Data Science.

2020–2021 Engagement in UChicago's Graduate Research Cooperative (GRC). Member of the committee that determines admissions to the PhD program.

2018–2019 Mentor for the Quantum Information Science and Engineering Network (QISE-NET), a NSF-funded national training program for graduate students pursuing careers in quantum science and engineering.

- **Organization of Conferences, Workshops and Meetups**

2022, Oct 13-14 Instructor and organizer, MICCoM Computational School, University of Chicago, https://miccom-center.uchicago.edu/workshop-and-hands-on-tutorials2022/index.html

2020, Dec 4 Organized the annual All-Hands meeting of the Midwest Integrated Center for Computational Materials, Argonne National Laboratory.

2019, Nov 4 Organized the annual All-Hands meeting of the Midwest Integrated Center for Computational Materials, Argonne National Laboratory.

2017, July 17-19 Instructor and co-organizer, MICCoM Computational School, University of Chicago, http://miccom-center.org/summer-school-2017/index.html

2017–2018 Early Career Network representative of the Energy Frontier Community. Organized National Meetups for young investigators.

- **Manuscript reviews**

  Science Advances, *Nature Light*, *Physical Review Letters*, *Physical Review Materials*, *Physical Review B*, *IOP Nanotechnology*, *AIP Advances*, *ACS Journal of Chemical Theory and Computation*, *AIP Journal of Chemical Physics*, *MDPI Materials*, *npj Computational Materials*, *International Journal of Quantum Chemistry*, *Chem Phys Chem*, *Carbon*, *Frontiers in Physics*.

- **Proposal reviews**

  – US Department of Energy/BES
  – US Department of Energy/FES
  – NSF
  – CINECA/ISCRA

Schools and Workshops Participation

2023, Jul 20 NVIDIA-Quantum Workshop, Oak Ridge National Lab, TN USA

2023, Jul 20	Quantinuum Workshop, Oak Ridge National Lab, TN USA
2023, Jul 17	IBM Workshop, Oak Ridge National Lab, TN USA
2023, Feb 27-Mar 3	Active Learning for Materials Science workshop 2023, Aalto University, Finland (virtual)
2022, Jul 18-29	Qiskit Global Summer School 2022 (virtual)
2021, Sept 22-23	OLCF & NERSC workshop, Introduction to OpenMP offloading for GPUs, Oak Ridge National Lab, TN (USA) (virtual)
2020, April 20, 27-29	Argonne GPU Hackathon, Argonne, Lemont, IL (USA) (virtual)
2020, Dec 8, 10	NVIDIA HPC SDK - OpenMP Target Offload Training, NERSC, Berkeley, CA (USA) (virtual)
2020, Sep 15-17	IBM Quantum Summit (USA) (virtual)
2019, Dec 4-6	NIST Scoping Workshop for the Research Data Management Framework (RDaF), NIST, Rockville MD, (USA)
2019, Nov 21-22	Materials Data Summit, Chicago IL, (USA)
2019, Jun 11-14	OPTiMaDe workshop: Open Databases Integration for Materials Design, Cecam, Lausanne, (Switzerland)
2018, Nov 12	Getting Started with Google Kubernetes Engine, RCC, University of Chicago, Chicago IL (USA)
2018, Oct 2-4	Simulation, Data, and Learning Workshop, ALCF, Argonne National Laboratory, Chicago IL (USA)
2018, Sep 12-14	Next Steps in Quantum Science for HEP, Fermilab, Batavia IL (USA)
2018, Feb 27-Mar 1	Simulation, Data, and Learning Workshop, ALCF, Argonne National Laboratory, Chicago IL (USA)
2016, Jul 31-Aug 12	*ATPESC-2016*, Argonne Training Program On Extreme-Scale Computing, St. Charles, IL (USA)
2016, Jun 21-Jul 28	*Academic and Professional Writing Class*, University of Chicago, Chicago IL (USA)
2015, May 19-21	*Mira Performance Boot Camp 2015*, ALCF, Argonne National Laboratory, Chicago IL (USA)
2014, May 20-22	*Mira Performance Boot Camp 2014*, ALCF, Argonne National Laboratory, Chicago IL (USA)
2012, Sep 26	*Techniques and tools for scientific programming on BlueGeneQ*, CINECA, Casalecchio di Reno (BO), Italy

2012, Feb 6-10 *PRACE Winter School: Hybrid programming on massively parallel architectures*, CINECA, Casalecchio di Reno (BO), Italy

2010, Dec 2-3 *Standard Formats for Scientific Data Management (HDF5, XML, Netcdf)*, CINECA, Casalecchio di Reno (BO), Italy

2010, Nov 29-Dec 1 *Python for Computational Science*, CINECA, Casalecchio di Reno (BO), Italy

2010, Oct 18-22 *Nanoexcite 2010*, Hands-on workshop on excitations in solids and nano-structures from first-principles, Sissa, Trieste, Italy

2010, May 17-28 *Spring College on Computational Nanoscience*, ICTP, Trieste, Italy

2010, Jan 02-15 *Time-Dependent Density-Functional Theory: Prospects and Applications*, 4^{th} International Workshop and School, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain

2009, Jul 06-17 *Summer School on Parallel Computing*, 18^{th} edition, CINECA, Casalecchio di Reno (BO), Italy

2008, May 13-17 *First principles molecular dynamics simulations in condensed matter and molecular physics*, Tutorial on Molecular dynamics, simulations using CPMD and CP2K packages, CECAM-ENS, Lyon, France

2006, Jun *Advanced courses on scientific programming: Fortran, C, C++, MPI*, CINECA, Casalecchio di Reno (BO), Italy

Outreach

2022 – present **IBM Qiskit Advocate**, *The Qiskit advocate program is a global program, run by IBM, that provides support to the individuals who actively contribute to the Qiskit software for quantum computing (https://qiskit.org/advocates/).*

2018 **Hour of code initiative**, *Led coding activities involving $\sim$ 150 elementary school students. Visited Schools:.*

- Fox Chase Elementary School, Oswego, Illinois (USA)
- Churchill Elementary School, Oswego, Illinois (USA)

Languages

English **Proficient** *Both written and oral*

Italian **Proficient** *Native*