Marco Govoni

Assistant Scientist, Argonne National Laboratory

Materials Science Division & Center for Molecular Engineering

9700 Cass Avenue
Building 241, room A381
Lemont, IL 60439 (USA)
+1 (530) 220 0081
mgovoni@anl.gov
www.marcogovoni.com

Current Position

2016–present **Assistant Scientist**, *Materials Science Division & Center for Molecular Engineering Argonne National Laboratory (IL), USA*.

- Modeling of materials for energy and quantum information science.
- Development and maintenance of scientific software for quantum simulations (http://www.west-code.org) and scientific data management (http://www.qresp.org).
- Member of the management team (directorate) of MICCoM, Computational Materials Science center funded by US Department of Energy/BES (http://miccom-center.org).

2018–present **Scientist**, *Consortium for Advanced Science and Engineering, The University of Chicago (IL), USA*.

- Supervision of students, post-doctoral researchers, and software/data engineers.

2019–present **Visiting Professor**, *Pritzker School of Molecular Engineering, The University of Chicago (IL), USA*.

- Teaching undergraduate and graduate courses.

Professional Experience

2014–2016 **Postdoc Research Scholar**, *Center for Molecular Engineering, Argonne National Laboratory & The University of Chicago, USA*.
Topic: Modeling Optoelectronic Properties of Materials. Supervisor: Prof. G. Galli.

2012–2014 **Postdoc Research Scholar**, *Dept. of Chemistry, University of California Davis, USA*.
Topic: Spectroscopy of Solids, Liquids, and Interfaces. Supervisor: Prof. G. Galli.

2012 **Postdoc Fellow**, *Italian Leadership Computing Facility CINECA, Casalecchio di Reno, Italy; and Dept. of Sciences and Methods for Engineering, University of Modena and Reggio Emilia, Italy*.
Topic: Modeling Solar-Energy Harvesting in Nanocompounds. Supervisors: Prof. S. Ossicini, Dr. I. Marri, Dr. C. Cavazzoni.

Education

2009–2012 **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.S. 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.S. 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.

Honors, Awards, and Qualifications

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

2019 Italian scientific qualification for professorship in Theoretical Physics of Condensed Matter (02/B2 sector; *seconda fascia*). Released by MIUR (Italian ministry for education, university and research). Validity: 2019–2028.

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 Computing Facility CINECA.

Career Highlights

- 33 peer-reviewed scientific publications. H-index: 15.
- Staff scientist at Argonne National Laboratory.
- Teaching undergraduate and graduate courses.
- PI and co-PI of several research grants, both as single investigator and collaborative.
- Recipient of the highly competitive DOE Early Career Award, with $2.5M research funding (https://science.osti.gov/early-career).
- Development of advanced computational techniques (based on density functional theory) for the advanced modeling of electron spectroscopies.
- Development and maintenance of scientific software for quantum simulations (http://www.west-code.org) and scientific data management (http://www.qresp.org).
- Consolidated experience in the computational characterization of complex systems of scientific and technological relevance.
- Formative and working experience in top-level international research centers and universities, including the University of California, the University of Chicago, and Argonne National Laboratory.

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 nanomaterials, renewable energy materials, water, and quantum information technologies

Molecular Engineering	Development of first principles approaches for materials property prediction
Scientific computing	Methodology and software development: massively scalable algorithms, parallel coding, GPUs, artificial intelligence, community codes, data repositories, reproducibility of scientific results
Quantum Computing	Development of hybrid classical-quantum algorithms for noisy intermediate-scale quantum computers

Reviewer Experience

Journals	*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*.
Funding agencies	*US Department of Energy/BES*, *US Department of Energy/FES*, *NSF*, *CINECA/ISCRA*

Organization of Conferences, Workshops and Meetups

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

Invited Talks and Seminars

2020, Aug 5	Intel seminar. *"Containers enabling interoperable environments in HPC"*
2020, Jul 29	Chicago Quantum Exchange briefing. *"Quantum simulations of materials on near-term quantum computers"*
2020, Jun 7-9	*GW-XL*, GW goes Large Scale, Aalto University, Helsinki, Finland. *"Large-scale Many-Body Perturbation Theory Calculations"*
2019, May 21-24	Tutorial on writing reproducible workflows for computational materials science, EPFL, Lausanne, Switzerland. *"Qresp, a tool for curating, discovering and exploring reproducible scientific papers"*
2018, Jun 11-15	Materials Genome Initiative at Exascale, Spetses, Greece. *"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. *"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. *"Multiscale modeling of materials interfaces at MICCoM and development of WEST"*

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

2017, May 30-31 Electrochemical Society Meeting, New Orleans, LA USA. *"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. *"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. *"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. *"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. *"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. *"Materials by design: methodological developments in the calculation of excited-state properties"*

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

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

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

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

Teaching

2019–2020 Visiting Professor. Instructor of the undergraduate and graduate course *Applied Scientific Computing in Molecular Engineering*, Pritzker School of Molecular Engineering, University of Chicago.

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

2015–2017 Lecturer. *Mathematical Foundation of Molecular Engineering*, held by Prof. Giulia Galli, Pritzker School of Molecular Engineering, University of Chicago

2011–2012 Teaching Assistant. *Quantum Mechanics*, held by Prof. Carlo Jacoboni, University of Modena and Reggio Emilia

2010–2011 Teaching Assistant. *Quantum Mechanics*, held by Prof. Carlo Jacoboni, University of Modena and Reggio Emilia

2009–2010 Teaching Assistant. *Quantum Mechanics*, held by Prof. Carlo Jacoboni, University of Modena and Reggio Emilia

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

Publications

Citation metrics are available on *Google Scholar* or *ORCID*.

- *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
- *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
- *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
- *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
- *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

- *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
- *Dielectric dependent hybrid functionals for heterogeneous materials*, H. Zheng, M. Govoni, and G. Galli, **Phys. Rev. Mat.** 3, 073803 (2019), DOI: 10.1103/PhysRevMaterials.3.073803
- *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
- *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
- *Optimizing oxide photo-absorbers: the role of defects and excess surface charges at finite temperature*, M. Gerosa, F. Gygi, M. Govoni, and G. Galli, **Nature Materials** 17, 1122 (2018), DOI: 10.1038/s41563-018-0192-4
- *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. Mat.** 2, 124002 (2018), DOI: 10.1103/PhysRevMaterials.2.124002
- *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
- *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
- *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
- *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
- *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. Materials** 14, 1700198 (2017), DOI: 10.1103/PhysRevMaterials.1.075002
- *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
- *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
- *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

- *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
- *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
- *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
- *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
- *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
- *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
- *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
- *Large scale GW calculations*, M. Govoni, and G. Galli, **J. Chem. Theory Comput.** 11, 2680 (2015), DOI: 10.1021/ct500958p
- *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
- *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
- *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
- *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
- *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

- *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 funding

PI: Principal Investigator.

PI *ECRP*, 2020 – present, "*Optical Control of Spin-polarization in Quantum Materials*", DOE Early Career Research Program (ECRP), Budget: \$500k/year. (https://science.osti.gov/early-career)

PI *ADSP*, 2019 – present, "*Advanced Materials Characterization with AI-Informed Computation*", Argonne Data Science Program (ADSP), Budget: two assigned staff scientists at Argonne National Leadership Computing Facility (ALCF).

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

PI *MICCoM-2*, 2019 – present "*Midwest Integrated Center for Computational Materials*", Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Budget: \$2.5M/year. Director of the center: G. Galli (http://miccom-center.org)

PI *LDRD*, 2019, "*Benchmark and Optimization of 3D-FFT Solvers for Many-Body Perturbation Theory Calculations*", ANL-LDRD research grant, Budget: \$32k.

PI *MICCoM-1*, 2015 – 2019 "*Midwest Integrated Center for Computational Materials*", Computational Materials Science Program funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Budget: \$3M/year. Director of the center: G. Galli (http://miccom-center.org)

PI *LDRD*, 2018, "*For Everyone A21: Distributed Electronic Structure Calculations Using A Globus-enabled Programmable Cyberinfrastructure*", ANL-LDRD research grant, Budget: \$25k

co-PI *ESP*, 2016 – 2018, "*Early Science Program Theta*", Research grant to get early access to the ANL-ALCF Theta machine. Budget: 1 fully funded postdoc and computational resources at ANL-ALCF. PI: G. Galli

PI 2010 – 2011, "*Ab initio calculations of out-of-equilibrium quasiparticle self-energies applied to highly excited Silicon Nanocrystals*", HPC research grant: HPC-EUROPA2, Budget: 6 Weeks paid short-term visit to Institute Néel, Grenoble, France

Projects

PI: Principal Investigator.

co-PI *ALCC2020*, "*Benchmarking Many-Body Perturbation Theory*", HPC research grant: ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy, Budget: 100k node h, PI: O. Heinonen

PI *ALCC2017*, "*Computational engineering of electron-vibration coupling mechanisms*", HPC research grant: ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy, Budget: 60M core h

PI *Nersc2017*, "*GW for the materials science community: extending transferability, benchmarking and addition of new productivity tools within the WEST code*", HPC research grant: NERSC, Budget: 3M core h

PI *ALCC2016*, "*Computational engineering of defects in soft and hard materials for energy and quantum information applications*", HPC research grant: ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy, Budget: 53.7M core h

PI *Nersc2016*, "*GW for the materials science community: extending transferability, benchmarking and addition of new productivity tools within the WEST code*", HPC research grant: NERSC, Budget: 3M core h

co-PI *Nersc2016*, "*Structure and stability of solids of nanoparticles from first principles*", HPC research grant: NERSC, Budget: 1M core h, PI: M. Handlin

co-PI *Nersc2016*, "*Large scale calculations on nanostructured heterogeneous interfaces*", HPC research grant: NERSC, Budget: 3M core h, PI: M. Vörös

PI *CNM2016*, "*Structure and stability of solids of nanoparticles from first principles*", HPC research grant: Center for Computational Nanomaterials, Budget: 0.87M core h

PI *LCRC2016*, "*GW for the materials science community*", HPC research grant, funded by the US Department of Energy, Budget: 1M core h

PI *ALCC2015*, "*First principles large scale simulations of interfaces for energy conversion and storage*", HPC research grant: ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy, Budget: 75M core h

PI *Nersc2015*, "*Ab-initio Photo-Electro-Chemical study of interfaces for water splitting*", HPC research grant: NERSC, Budget: 2M core h

co-PI *Larnint2015*, "*Large scale calculations on nanostructured heterogeneous interfaces*", HPC research grant: NERSC-NISE, Budget: 2M core h, PI: M. Vörös

co-PI 2014, *MEGAPV*, "*Multiple Exciton Generation: Application to PhotoVoltaic*", HPC research grant: Prace 8th call, Budget: 32M core h, PI: S. Ossicini

co-PI 2014, *TOWER-NY*, "*simulaTiOn of neW carriER multiplication mechanisms in silicon NanocrYstals*", HPC research grant: Cineca-ISCRA B, Budget: 7.8M core h, PI: I. Marri

co-PI 2014, *Larnint2014*, "*Large scale calculations on nanostructured heterogeneous interfaces*", HPC research grant: NERSC-NISE, Budget: 5M core h, PI: M. Vörös

co-PI 2013, *MOMA-NY*, "*Multiexcitons at a cOst of one: carrier MultiplicAtion in silicon NanocrYstals*", HPC research grant: Cineca-ISCRA A, Budget: 8M core h, BG/Q Fermi, PI: I. Marri

co-PI 2012, *HOTSUN*, "*High perfOrmance compuTing in Silicon nanostructrUres for third generatioN photovoltaics*", HPC research grant: Prace 5th call, Budget: 10.5M core h, BG/Q Fermi, PI: S. Ossicini

PI 2011, *MEGINSUN*, "*Multiple Exciton Generation in Si nanostrUctures for photovoltaic applicatioNs*", HPC research grant: Cineca-ISCRA B, Budget: 150k core h

PI 2011, *FARESSSN*, "*Fast-recombination by Surface States in Silicon Nanocrystals*", HPC research grant: Cineca-ISCRA C, Budget: 48k core h

PI 2011, *PHOSSI*, "*PHOnon Spectra in SI nanocrystals*", HPC research grant: Cineca-ISCRA C, Budget: 20k core h

PI 2011, "*Auger Recombination in Silicon Nano-Crystals*", HPC research grant: CASPUR-Standard grant, Budget: 63k core h

PI 2010, *COSENANO*, "*Ab initio Calculations of Out-of-equilibrium quasiparticle SElf energies applied to highly excited Silicon NANOcrystals*", HPC research grant: Cineca-ISCRA C, Budget: 20k core h

PI 2010, *CAMUSI*, "*Carrier Multiplication in Si-nanostructures*", HPC research grant: Cineca-ISCRA C, Budget: 20k core h

Contributions at Conferences

2019, Mar 31-Apr 4 *ACS 2019*, Annual National 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)

2016, Mar 14-18 *APS March Meeting 2016*, Annual Meeting of the American Physical Society, Baltimore, MD USA. **Talk** "Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids", **Talk** "Solvated ions as defects in liquid water: A first-principles perspective", **Talk** "Photoemission spectra of aqueous solutions of salts from many-body perturbation theory", **Talk** "A non-empirical, parameter-free, hybrid functional for accurate calculations of optoelectronic properties of finite systems"

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", **Talk** "Using Dielectric Properties to Design Nonempirical Hybrid Functionals for Accurate Electronic Structure", **Talk** "First-principles theory of defect spins in w-AlN for quantum information and sensing technologies", **Talk** "Faster GW total energy calculations"

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", **Talk** "A Self-consistent Mixing Parameter Scheme for Hybrid Functionals Applied to Periodic 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", **Talk** "Carrier Multiplication Effects Between Interacting Nanocrystals for Solar Cell Applications"

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"

Schools and Workshops

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

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	**Excellent**	*Both written and oral*
Italian	**Excellent**	*Native*
German	**Intermediate**	
Japanese	**Elementary**	*4th level of JLPT*

Skills

Scientific Development of models and applications in Materials Science, Computer Science, and Data Science. Proposal writing. Scientific management. Personnel supervision. Teaching at undergraduate and graduate level, and training of personnel.

Computational Programming languages: Python, Fortran, C, C++, HTML, Java. Experience with high-performace computing facilities (NERSC, ALCF, OLCF, CINECA), extensive knowledge of MPI and OpenMPI. Frameworks and Tools: Git, Tensorflow, Numpy, Matplotlib, Pandas, Jupyter-notebook, Containers (Docker, Singularity).

Personal Problem-solving. Excellent communication skills (both written and oral). Ability to take initiative, and to work independently in an organized manner prioritizing the work of multiple projects. Ability to work collegially and as part of a team. Ability to manage a large volume of work often restricted by deadlines. Ability to use appropriate resources to resolve an issue.

References

- **Prof. Giulia Galli**, The University of Chicago, Pritzker School of Molecular Engineering, 5640 South Ellis Avenue, Chicago IL 60637 USA, phone: +1 773-702-0515, email: gagalli@uchicago.edu
- **Prof. Francois Gygi**, University of California Davis, Department of Computer Science, 3013 Ghausi Hall (Engineering III), Davis, CA 95616 USA, phone: +1 530-752-4042, email: fgygi@ucdavis.edu
- **Prof. Stefano Ossicini**, University of Modena and Reggio Emilia, Dipartimento di Scienze e Metodi dell'ingegneria, Via Amendola 2 (padiglione Morselli), 42100 Reggio Emilia, Italy, phone: +39 0522-522-211, email: stefano.ossicini@unimore.it
- **Prof. Carlo Calandra Buonaura**, University of Modena and Reggio Emilia, Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Via Campi 213/A, 41125 Modena, Italy, phone: +39 059-205-5290, email: carlo.calandrabuonaura@unimore.it
- **Dr. Carlo Cavazzoni**, CINECA, Supercomputing Applications and Innovation, Via Magnanelli 6/3, 40033 Casalecchio di Reno, Bologna, Italy, phone: +39 051-6171-595, email: c.cavazzoni@cineca.it
- **Dr. Ivan Marri**, University of Modena and Reggio Emilia, Dipartimento di Scienze e Metodi dell'ingegneria, Via Amendola 2 (padiglione Morselli), Italy, phone: +39 059-205-5067, email: ivan.marri@unimore.it