

ALLEGATO B

UNIVERSITÀ DEGLI STUDI DI MILANO

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Marco Govoni CURRICULUM VITAE

INFORMAZIONI PERSONALI (NON INSERIRE INDIRIZZO PRIVATO E TELEFONO FISSO O CELLULARE)

COGNOME	GOVONI
NOME	MARCO
DATA DI NASCITA	04/02/1984

**INSERIRE IL PROPRIO CURRICULUM
(non eccedente le 30 pagine)**

Data

14/09/2020

Luogo

CHICAGO (USA)

Marco Govoni

*Assistant Scientist, Argonne National Laboratory
Materials Science Division & Center for Molecular Engineering*

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Posizione attuale

- 2016–
presente **Assistant Scientist**, *Materials Science Division & Center for Molecular Engineering Argonne National Laboratory (IL), USA.*
- Partecipazione a progetti di ricerca aventi come scopo la modellizzazione di materiali attraverso simulazioni quantistiche.
 - Sviluppo e mantenimento di software open-source per: simulazioni quantistiche (<http://www.west-code.org>), gestione e diffusione di dati scientifici (<http://www.qresp.org>).
 - Organizzazione, direzione e coordinamento di gruppi di ricerca. Membro del gruppo dirigente del centro di ricerca MICCoM (<http://miccom-center.org>), finanziato dal U.S. Department of Energy.
 - Supervisione di ricercatori (postdocs).
- 2018–
presente **Scientist**, *Consortium for Advanced Science and Engineering, The University of Chicago (IL), USA.*
- Supervisione di studenti, postdocs ed ingegneri informatici.
- 2019–
presente **Visiting Professor**, *Pritzker School of Molecular Engineering, The University of Chicago (IL), USA.*
- Docente di corsi di laurea e di dottorato.

Esperienza professionale

- 2014–2016 **Postdoc**, *Materials Science Division & Center for Molecular Engineering, Argonne National Laboratory & The University of Chicago, USA.*
Tema: Modellizzazione di proprietà optoelettroniche dei materiali. Supervisore: Prof. G. Galli.
- 2012–2014 **Postdoc**, *Dept. of Chemistry, University of California Davis, USA.*
Tema: Spettroscopia di Solidi, Liquidi, e Interfacce. Supervisore: Prof. G. Galli.
- 2012 **Postdoc**, *CINECA, Casalecchio di Reno, Italia; e Dipartimento di Scienze e Metodi per l'Ingegneria, Università di Modena e Reggio Emilia, Italia.*
Tema: Modellizzazione di materiali nanostrutturati per celle solari. Supervisor: Prof. S. Ossicini, Dr. I. Marri, Dr. C. Cavazzoni.

Istruzione

- 2009–2012 **Dottorato di ricerca in Nanoscienze e Nanotecnologie**, *Università di Modena e Reggio Emilia, Italia.*
Tesi: “Coulomb-driven recombinations in semiconductors: from bulk to nanocrystals”. Relatori: Prof. S. Ossicini e Dr. I. Marri.

- 2006–2008 **Laurea Specialistica in Fisica**, *Università di Modena e Reggio Emilia, Italia*.
Voto: 110/110 e lode. Tesi: “*Role and applications of the vacuum force in microscopic systems*”. Relatore: Prof. C. Calandra Buonauro.
- 2003–2006 **Laurea Triennale in Fisica**, *Università di Modena e Reggio Emilia, Italia*.
Voto: 110/110 e lode. Tesi: “*Ab-initio simulations of STM images*”. Relatori: Prof. G. Goldoni, Dr. A. Calzolari, Dr. C. Cavazzoni.

Premi e abilitazioni

- 2020 Premio *DOE Early Career Award*, conferito da U.S. Department of Energy, Office of Science, Basic Energy Sciences, sezione di Theoretical Condensed Matter Physics. Accesso tramite competizione nazionale.
- 2019 Abilitazione scientifica nazionale in Fisica Teorica della Materia (settore concorsuale 02/B2; *seconda fascia*), rilasciata dal Ministero Italiano della Istruzione, della Università e della Ricerca (MIUR). Validità: 2019–2028.
- 2016 Japan Society for the Promotion of Science (JSPS) invitation fellowship.
- 2015 Premio *Best Scalable Software*, Mind the Bytes, University of Chicago.
- 2012 Borsa di post-dottorato ISCR, conferita dal consorzio interuniversitario CINECA (Italia). Accesso tramite competizione nazionale.

Sintesi della carriera

- 33 pubblicazioni scientifiche. H-index: 15.
- Ricercatore permanente presso Argonne National Laboratory.
- Docente di corsi di laurea e di dottorato a studenti di Ingegneria, Fisica e Chimica.
- Principal Investigator (PI) di diversi progetti di ricerca, sia come *single investigator* sia in collaborazione.
- Ricevente del premio di ricerca altamente competitivo DOE Early Career award, con finanziamento di \$2.5M (<https://science.osti.gov/early-career>).
- Sviluppo di tecniche computazionali (basate sulla teoria del funzionale densità) per la modellizzazione avanzata di spettroscopie elettroniche.
- Sviluppo e mantenimento di software scientifici per simulazioni quantistiche (<http://www.west-code.org>), gestione e diffusione di dati scientifici (<http://www.qresp.org>).
- Esperienza consolidata in caratterizzazione computazionale di sistemi complessi di rilevanza scientifica e tecnica.
- Esperienza formativa e lavorativa presso enti di ricerca ed università internazionali: University of California, University of Chicago, Argonne National Laboratory.

Interessi di ricerca

Marco è un fisico della materia con esperienza in progetti multidisciplinari in fisica, chimica, matematica, scienza dell'informazione e dei dati. Ha sviluppato tecniche di modellizzazione basate su simulazioni da

principi primi, al fine di predire le proprietà di materiali per studi avanzati relativi a energie rinnovabili, sistemi liquidi, e informazione quantistica.

Simulazioni quantistiche	Modellizzazione atomistica da principi primi di nanomateriali, materiali per energie rinnovabili, sistemi liquidi, e informazione quantistica
Ingegneria molecolare	Sviluppo di tecniche e metodi per la predizione di proprietà di materiali da principi primi
Calcolo scientifico	Sviluppo di software scientifico: algoritmi paralleli, GPUs, intelligenza artificiale, codici open-source, archiviazioni di dati scientifici, riproducibilità dei dati scientifici
Calcolo quantistico	Sviluppo di algoritmi ibridi classici-quantum per computer quantistici (noisy intermediate-scale quantum computers)

Esperienza come revisore scientifico

Riviste	<i>Science Advances, Nature Light, Physical Review Letters, Physical Review B, Physical Review Materials, 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.</i>
Enti di ricerca	<i>US Department of Energy/BES, US Department of Energy/FES, NSF, CINECA/ISCRA</i>

Organizzazione di conferenze ed eventi scientifici

2019, Nov 4	Organizzatore del All-Hands meeting annuale del Midwest Integrated Center for Computational Materials, Argonne National Lab.
2017, Lug 17-19	Istruttore e co-organizzatore, Scuola Computazionale MICCoM, University of Chicago, http://miccom-center.org/summer-school-2017/index.html
2017–2018	Membro del Early Career Network della Energy Frontier Community. Organizzazione di National Meetups tra giovani ricercatori.

Lista di inviti come oratore a seminari o convegni scientifici

2020, Ago 5	Intel, seminario. “Containers enabling interoperable environments in HPC”
2020, Lug 29	Chicago Quantum Exchange briefing. “Quantum simulations of materials on near-term quantum computers”
2020, Giu 7-9	GW-XL, GW goes Large Scale, Aalto University, Helsinki, Finlandia. “Large-scale Many-Body Perturbation Theory Calculations”
2019, Mag 21-24	Tutorial on writing reproducible workflows for computational materials science, EPFL, Losanna, Svizzera. “Qresp, a tool for curating, discovering and exploring reproducible scientific papers”
2018, Giu 11-15	Materials Genome Initiative at Exascale, Spetses, Grecia. “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, Gen 17 High Performance Computing for Manufacturing, Argonne National Lab, IL USA. *"Multiscale modeling of materials interfaces at MICCoM and development of WEST"*
- 2017, Dic 21 Seminario, Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, Modena, Italia. *"Large Scale Many-Body Perturbation Theory Calculations: Software, Data and Applications"*
- 2017, Ott 19 Seminario, Department of Physics, Central Michigan University, Mt. Pleasant, MI USA. *"Large Scale Many-Body Perturbation Theory Calculations: Software, Data and Applications"*
- 2017, Mag 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, Gen 12-14 18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, ICTP, Trieste, Italia. *"Large Scale Many-Body Perturbation Theory Calculations: Methodological Developments, Data Collections, Validation and Applications"*
- 2016, Ott 24-28 OPTIMADE Workshop: Open Databases Integration for Materials Design, Lorentz Center, Leiden, Olanda. *"Midwest Integrated Center for Computational Materials (MICCoM): Software, Validation & Data"*
- 2016, Ago 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, Gen 18-21 QuantumESPRESSO developers meeting, ICTP, Trieste, Italia. *"WEST: open source software for accurate electronic structure simulations"*
- 2015, Dic 18 Physics in Modena 2015, Annual meeting of the Università di Modena e Reggio Emilia alumni, Modena, Italia. *"From punched cards to modern HPC supercomputers: electronic structure methods"*
- 2015, Set 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, Ago 10-14 248th ACS National Meeting & Exposition, San Francisco, CA USA. *"Photoexcitations in semiconductors and insulators from first principles"*

Attività didattica

- 2019–2020 Docente del corso di laurea *Applied Scientific Computing in Molecular Engineering*, Pritzker School of Molecular Engineering, University of Chicago.
- 2017 Istruttore ed organizzatore della *Scuola Computazionale MICCoM*, Pritzker School of Molecular Engineering, University of Chicago.
- 2011–2012 Assistente alla didattica. *Meccanica Quantistica*, corso di laurea tenuto da Prof. C. Jacoboni, Università di Modena e Reggio Emilia
- 2010–2011 Assistente alla didattica. *Meccanica Quantistica*, corso di laurea tenuto da Prof. C. Jacoboni, Università di Modena e Reggio Emilia
- 2009–2010 Assistente alla didattica. *Meccanica Quantistica*, corso di laurea tenuto da Prof. C. Jacoboni, Università di Modena e Reggio Emilia

Visite scientifiche

- 2016 Nov-Dic National Institute for Materials Science, Tsukuba, Giappone, presso: Prof. Ikutaro Hamada. Visita finanziata dalla società giapponese per la promozione della scienza.
- 2010 Giu-Lug Institute Néel, Grenoble, Francia, presso: Dr. Claudio Attaccalite. Visita finanziata dalla Comunità Europea.

Pubblicazioni

Contatori bibliografici consultabili presso *Google Scholar* o *ORCID*.

- *First-principles Studies of Strongly Correlated States in Defect Spin Qubits in Diamond*, H. Ma, N. Sheng, M. Govoni, and G. Galli, submitted (2020), ArXiv: 2008.13283
- *Coupling interoperable software for quantum simulations of materials*, M. Govoni, J. Whitmer, J. de Pablo, F. Gygi, and G. Galli, submitted (2020)
- *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
- *MatD³: 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

Fondi di ricerca

PI: Principal Investigator.

- PI *ECRP*, 2020 – presente, “*Optical Control of Spin-polarization in Quantum Materials*”, DOE Early Career Research Program (ECRP), Budget: \$500k/anno. (<https://science.osti.gov/early-career>)
- PI *ADSP*, 2019 – presente, “*Advanced Materials Characterization with AI-Informed Computation*”, Argonne Data Science Program (ADSP), Budget: 2 assigned staff scientists at Argonne National Leadership Computing Facility (ALCF).
- PI *NESAP*, 2019 – presente, “*Many-Body Perturbation Theory with WEST*”, NERSC Exascale Science Application Program (NESAP) Tier 1 research project, Budget: 1 postdoctoral researcher at U.S. National Energy Research Scientific Computing (NERSC).
- PI *MICCoM-2*, 2019 – presente “*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/anno. Direttrice del centro: 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/anno. Direttrice del centro: 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

Progetti

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

Conferenze

- 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, Giu 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, Mag 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, Gen 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, Gen 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, Lug 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, Set 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, Set 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, Set 27-30 *ETSF-2011*, 16th ETSF Workshop on Electronic Excitations, Turin, Italy. **Talk** "Auger Recombination and Impact Ionization from first-principles: from bulk to nanocrystals"
- 2011, Mag 16-20 *YRM11*, 8th 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, Gen 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, Set 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, Set 21-25 *QFEXT09*, 9th 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, Giu 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, Giu 2-6 *YRM09*, 6th 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"

Scuole e workshops

- 2019, Dic 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, Giu 11-14 OPTiMaDe workshop: Open Databases Integration for Materials Design, Cecam, Losanna, (Svizzera)
- 2018, Nov 12 Getting Started with Google Kubernetes Engine, RCC, University of Chicago, Chicago IL (USA)
- 2018, Ott 2-4 Simulation, Data, and Learning Workshop, ALCF, Argonne National Laboratory, Chicago IL (USA)
- 2018, Set 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, Lug 31-Aug 12 *ATPESC-2016*, Argonne Training Program On Extreme-Scale Computing, St. Charles, IL (USA)
- 2016, Giu 21-Lug 28 *Academic and Professional Writing Class*, University of Chicago, Chicago IL (USA)

- 2015, Mag 19-21 *Mira Performance Boot Camp 2015*, ALCF, Argonne National Laboratory, Chicago IL (USA)
- 2014, Mag 20-22 *Mira Performance Boot Camp 2014*, ALCF, Argonne National Laboratory, Chicago IL (USA)
- 2012, Set 26 *Techniques and tools for scientific programming on BlueGeneQ*, CINECA, Casalecchio di Reno (BO), Italia
- 2012, Feb 6-10 *PRACE Winter School: Hybrid programming on massively parallel architectures*, CINECA, Casalecchio di Reno (BO), Italia
- 2010, Dic 2-3 *Standard Formats for Scientific Data Management (HDF5, XML, Netcdf)*, CINECA, Casalecchio di Reno (BO), Italia
- 2010, Nov 29-Dec 1 *Python for Computational Science*, CINECA, Casalecchio di Reno (BO), Italia
- 2010, Ott 18-22 *Nanoexcite 2010*, Hands-on workshop on excitations in solids and nano-structures from first-principles, Sissa, Trieste, Italia
- 2010, Mag 17-28 *Spring College on Computational Nanoscience*, ICTP, Trieste, Italia
- 2010, Gen 02-15 *Time-Dependent Density-Functional Theory: Prospects and Applications*, 4th International Workshop and School, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spagna
- 2009, Lug 06-17 *Summer School on Parallel Computing*, 18th edition, CINECA, Casalecchio di Reno (BO), Italia
- 2008, Mag 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, Lione, Francia
- 2006, Giu *Advanced courses on scientific programming: Fortran, C, C++, MPI*, CINECA, Casalecchio di Reno (BO), Italia

Divulgazione scientifica

2018 **Iniziativa Hour of code**, Diretto attività di sviluppo di codice coinvolgendo ~ 150 alunni di scuole elementari.

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

Lingue

Inglese	Eccellente	<i>Sia scritto che orale</i>
Italiano	Eccellente	<i>Madrelingua</i>
Tedesco	Intermedio	
Giapponese	Base	<i>4to livello JLPT</i>

Conoscenze

- Scientifiche** Sviluppo di modelli ed applicazioni di fisica, chimica, matematica, scienza dell'informazione e dei dati. Scrittura di progetti. Management di progetti. Supervisione di personale. Didattica a studenti di Ingegneria, Fisica e Chimica.
- Computazionali** Linguaggi di programmazione: Python, Fortran, C, C++, HTML, Java. Esperienza con high-performace computing facilities (NERSC, ALCF, CINECA). Frameworks e Tools: Git, Tensorflow, OpenMP, MPI, Numpy, Matplotlib, Pandas, Jupyter-notebook, Containers (Docker, Singularity).
- Personali** Problem-solving. Ottime capacità di comunicazione (sia scritte che orali). Capacità di prendere iniziativa, e di lavorare in autonomia in modo organizzato ed assegnando priorità a molteplici progetti eseguiti simultaneamente. Capacità di lavorare in gruppo o in collaborazioni. Capacità di gestire un grande volume di lavoro in presenza di deadlines. Capacità di allocare le risorse appropriate per risolvere un problema.

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