ALLEGATO B

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Marco Govoni
CURRICULUM VITAE

INFORMAZIONI PERSONALI

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

Data 29/07/2019 Luogo Chicago (USA)

Marco Govoni

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

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Building 241, room A381
Lemont, IL 60439 (USA)
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Posizione attuale

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

- Modellizzazione di materiali attraverso simulazioni quantistiche.
- Sviluppo e mantenimento di software open-source per simulazioni quantistiche (http://www.west-code.org) e gestione di dati scientifici (http://www.qresp.org).
- Membro del gruppo dirigente del centro di ricerca MICCoM, finanziato dal dipartimento dell'energia degli Stati Uniti d'America (http://miccom-center.org).

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

- Supervisione di studenti, ricercatori e di ingegneri informatici.

Esperienza professionale

2014–2016 **Postdoc**, *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. Supervisori: Prof. S. Ossicini, Dr. I. Marri, Dr. C. Cavazzoni.

Istruzione

2009–2012 **Dottorato di ricerca in Nanoscienze e Nanotechnologie**, *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 Buonaura.

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

2019 Abilitazione scientifica nazionale in Fisica Teorica della Materia (settore concorsuale 02/B2; *seconda fascia*), rilasciato dal Ministero Italiano della Istruzione, della Università e della Ricerca (MIUR). Validità: 2019–2025.

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

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

2012 ISCRA borsa di post-dottorato, Italian Leadership Computing Facility CINECA. Accesso tramite competizione nazionale.

Sintesi della carriera

- 28 pubblicazioni scientifiche. H-index: 15.
- Staff scientist presso Argonne National Laboratory.
- PI e co-PI di diversi progetti di ricerca finanziati da enti americani (Department of Energy, DoE).
- Sviluppo di tecniche computazionali (basate sulla teoria del funzionale densità) per la modellizzazione avanzata di spectroscopie elettroniche.
- Sviluppo e mantenimento di software scientifico per simulazioni quantistiche (http://www.west-code.org) e gestione dei dati scientifici (http://www.qresp.org).
- Esperienza consolidata in caratterizzazione computazionale di sistemi complessi di rilevanza scientifica e tecnica.
- Esperienza formativa e lavorativa presso gruppi di ricerca ed università internazionali: University of California, e University of Chicago.

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, codici open-source, archiviazioni di dati scientifici, riproducibilità dei dati scientifici

Esperienza come revisore scientifico

Riviste *Science Advances*, *Nature Light*, *Physical Review Letters*, *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*.

Enti di ricerca *US Department of Energy/BES*, *US Department of Energy/FES*, *CINECA/ISCRA*

Organizzazione di conferenze ed eventi scientifici

2017, Lug 17-19 Istruttore e co-organizzatore, Scuola Computazionale MICCoM, University of Chicago, http://miccom-center.org/summer-school-2017

2017–2018 Membro del Early Career Network del Energy Frontier Community. Organizzazione di National Meetups tra giovani ricercatori.

Lista di inviti come oratore a seminari o convegni scientifici

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 Seminar, Department of Physics, Informatics and Mathematics, 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

2017 Istruttore. *Scuola Computazionale MICCoM*, Pritzker School of Molecular Engineering, University of Chicago. Organizzato sessioni didattiche

2015–2017 Assistente alla didattica. *Mathematical Foundation of Molecular Engineering*, corso tenuto dalla Prof. G. Galli, Pritzker School of Molecular Engineering, University of Chicago

2009–2012 Assistente alla didattica. *Meccanica Quantistica*, corso tenuto dal Prof. C. Jacoboni, Departimento di Fisica, Università di Modena e Reggio Emilia

Visite scientifiche

2016 Nov-Dic National Institute for Materials Science, Tsukuba, Giappone, presso: Prof. Ikutaro Hamada

2010 Giu-Lug Institute Néel, Grenoble, Francia, presso: Dr. Claudio Attaccalite

Pubblicazioni

Contatori bibliografici consultabili presso *Google Scholar*

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

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).

co-PI *MICCoM*, 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/year. PI: G. Galli

co-PI *MICCoM*, 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. PI: G. Galli

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 *ALCC2017*, "*Computational engineering of electron-vibration coupling mechanisms*", HPC research grant: ASCR Leadership Computing Challenge (ALCC), funded by the US Department of Energy, Budget: 75M 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, CA 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 Reseach 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*, 16^{th} 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*, 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, 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*, 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, 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*, 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"

Scuole e workshops

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*, 4^{th} International Workshop and School, Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spagna
2009, Lug 06-17	*Summer School on Parallel Computing*, 18^{th} 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**, *Condotto 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**	*Sia scritto che orale*
Italiano	**Eccellente**	*Madrelingua*
Tedesco	**Intermedio**	
Giapponese	**Base**	*4to livello JLPT*

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