Marco Govoni

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Institute for Molecular Engineering & Materials Science Division

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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	Electronic excited states of solids, surfaces, interfaces and nanostructures, Density Functional Theory (DFT), Many Body Perturbation Theory (MBPT), Computational spectroscopy
Scientific computing	Software development and maintenance, massively scalable algorithms, community codes, data repositories, reproducibility of scientific results
Molecular Engineering	Quantum dots, nanocrystals, band alignment at interfaces, aqueous solutions, carrier recombinations, exciton dynamics, charge and energy transfer
Applications	Materials for energy, photovoltaics, photocatalysis, quantum information

Professional Experience

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

- Part of the management team (directorate) of MICCoM, Computational Materials Science center funded by US Department of Energy/BES (http://miccom-center.org)
- Development and maintenance of scientific software for quantum simulations (http://www.west-code.org) and scientific data management (http://www.qresp.org)
- First-principles simulations of materials for renewable energies and quantum information
- Supervision of a team of undergraduate and graduate students, and post-doctoral research assistants dedicated to developing methods for ab-initio simulations

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

2012–2014 **Postdoc Research Scholar**, *Department of Chemistry, University of California Davis, Davis, (CA) USA*.
Topic: Electron Spectroscopies of Solids, Liquids, Interfaces and Nanostructures
Supervisor: Prof. G. Galli

2012 **Postdoc Fellow**, *Italian Leadership Computing Facility CINECA, Casalecchio di Reno (BO), Italy*.
Topic: Modeling of Solar-Energy Harvesting in Nanocompounds
Supervisors: Prof. S. Ossicini, Dr. I. Marri, Dr. C. Cavazzoni

Honors and Awards

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

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

2012 ISCRA postdoctoral fellowship, Italian Leadership Computing Facility CINECA

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"*
Supervisors: Prof. S. Ossicini and Dr. I. Marri

2006–2008 **M.S. Physics**, *University of Modena and Reggio Emilia, Italy*, *110/110 cum laude*.
Thesis: *"Role and applications of the vacuum force in microscopic systems"*
Supervisor: Prof. C. Calandra Buonaura

2003–2006 **B.S. Physics**, *University of Modena and Reggio Emilia, Italy*, *110/110 cum laude*.
Thesis: *"Ab-initio simulations of STM images"*
Supervisors: Prof. G. Goldoni, Dr. A. Calzolari, Dr. C. Cavazzoni

Reviewer Experience

Journals *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*.

Funding agencies *US Department of Energy/BES*, *CINECA/ISCRA*

Organization of Conferences and Meetups

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

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

Invited Talks and Seminars

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, 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

2017 Instructor. *MICCoM Computational School*, Institute for Molecular Engineering, University of Chicago, Organized hands-on sessions

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

2009–2012 Teaching Assistant. *Quantum Mechanics*, held by Prof. Carlo, Department of Physics, 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

- *Qresp: curation and exploration of reproducible scientific papers*, **M. Govoni**, M. Munakami, A. Tanikanti, J. Skone, H. Runesha, F. Giberti, J. de Pablo, and G. Galli, submitted (2018)
- *A finite field approach to solve the Bethe Salpeter equation*, N. L. Nguyen, H. Ma, **M. Govoni**, F. Gygi, and G. Galli, submitted (2018)
- *Optimizing oxide photo-absorbers: the role of defects and excess surface charges at finite temperature*, M. Gerosa, F. Gygi, **M. Govoni**, and G. Galli, submitted (2018)
- *Combined First Principles Calculations of Electron-Electron and Electron-Phonon Scattering*, R. McAvoy, **M. Govoni**, and G. Galli, submitted (2018)
- *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

Grants

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

co-PI *ESP2016*, "*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 *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, "*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

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

2018, Mar 5-9 *APS March Meeting 2018*, Annual Meeting of the American Physical Society, Los Angeles, CA USA. **Oral** "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. **Oral** "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. **Oral** "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. **Oral** "Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids", **Oral** "Solvated ions as defects in liquid water: A first-principles perspective", **Oral** "Photoemission spectra of aqueous solutions of salts from many-body perturbation theory", **Oral** "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. **Oral** "High performance electronic structure engineering"

2015, Mar 2-6 *APS March Meeting 2015*, Annual Meeting of the American Physical Society, San Antonio, TX USA. **Oral** "High performance electronic structure engineering", **Oral** "Using Dielectric Properties to Design Nonempirical Hybrid Functionals for Accurate Electronic Structure", **Oral** "First-principles theory of defect spins in w-AlN for quantum information and sensing technologies", **Oral** "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. **Oral** "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. **Oral** "Computing quasiparticle energies and band offsets for large systems", **Oral** "A Self-consistent Mixing Parameter Scheme for Hybrid Functionals Applied to Periodic Systems"

2013, Jul 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. **Oral** "Computational spectroscopy of nanocomposites", **Oral** "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. **Oral** "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. **Oral** "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. **Oral** "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. **Oral** "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

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

Languages

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

References

- **Prof. Giulia Galli**, The University of Chicago, Institute for Molecular Engineering, 5640 South Ellis Avenue, Chicago IL 60637 USA, phone: +1 773-702-0515, email: gagalli@uchicago.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), 42100 Reggio Emilia, Italy, phone: +39 059-205-5067, email: marri@unimo.it