Matteo Cococcioni

Researcher ID: L-5955-2013

Contacts:

Room 2-02, Physics Department,
University of Pavia,
Via Bassi 6, I-27100 Pavia

Email: matteo.cococcioni@unipv.it
Phone: +39 0382 987485

CURRENT POSITION

2018 – present	Senior (tenure-track) researcher Physics Department, University of Pavia, Pavia, Italy

SCIENTIFIC DEGREES

1999 – 2002	Ph.D. in Physics. Condensed Matter sector of the International School for Advanced Studies (SISSA-ISAS), Trieste, Italy. Thesis: "*A LDA+U study of selected iron compounds*". Advisor: Prof. Stefano de Gironcoli
1994 – 1999	Laurea in Physics. Department of Physics "A. Volta" of the University of Pavia, Italy. Thesis: "*Variational study of a dimer with a complete set of electronic and phononic interactions*". Grade: 110/110 with honors. Advisors: Profs A. Rigamonti (University of Pavia) and M. Acquarone (CNR, University of Parma).

PROFESSIONAL EXPERIENCE

2013 – 2018	Senior Scientist. Theory and Simulation of Materials, Institute of Materials, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
2006 – 2013	Assistant professor. Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, USA
2003 – 2006	Postdoctoral research assistant. Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA

ABILITATIONS

Italian "scientific abilitation" as associate and full professor in Theoretical Physics of Condensed Matter (02/B2 sector). Released by MIUR (Italian ministry for education, university and research). Validity: 2018 – 2024.

CAREER HIGHLIGHTS
Important achievements, experiences and competences

- 52 publications on peer-reviewed scientific journals or on-line archives; 3 non peer-reviewed publications (including chapters on books); 1 conference proceedings. H-index: 27 (30); 14662 (19003) citations; average number of citations per article: 303 (393). Source: ISI Web of Science (Google Scholar), June 2019
- Assistant professor at the University of Minnesota: definition and direction of a research program through the formation and coordination of an independent group; teaching at both undergraduate and graduate (master and PhD) levels
- Obtained several research grant from European and American funding agencies, including the US National Science Foundation (NSF) and the US Department of Energy (DOE)
- CAREER award from the Department of Materials Research of the US NSF
- Development of advanced computational techniques (based on density functional theory – DFT) for the accurate modeling of systems characterized by strong electronic localization
- Consolidated experience in the computational characterization of complex systems of scientific and technological relevance
- Formative and working experience in top level international research groups and institutes including the International School for Advanced Studies (SISSA – ISAS) of Trieste, Italy, the Massachusetts Institute of Technology (MIT) of Cambridge, USA, and the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland
- Residency at the Collegio Ghislieri of Pavia during the undergraduate studies in Physics (1994 – 1999). The position was obtained by a selective entrance exam and maintained by excellence of university records (27/30 minimum average grade, with no grade below 24/30 in any course)

RESEARCH EXPERIENCE AND INTERESTS

My scientific activity focuses on the modeling, based on first-principles computational techniques, of materials of scientific relevance and technological interest, with particular focus on transition-metal compounds. The research work I have developed through my career, encompasses the study of a broad variety of systems, including materials for Li-ion batteries, semiconductor nanoparticles, materials for thin film solar cells, magnetic shape-memory alloys, materials with high magnetization density, transition-metal minerals of the Earth's mantle, transparent conductive oxides, sensitizing complexes used as dyes for organic solar cells, catalytic systems hosted in porous crystals (zeolites and metal-organic frameworks) for the synthesis, purification and conversion of liquid and gas fuels. Besides their technological relevance, these systems have attracted my interest for the importance that electronic correlations have in determining their properties and behavior. In fact, a very relevant part of my work also hinges around the development of advanced corrective functionals able to improve the accuracy of current approximations to density-functional theory (DFT) in the modeling of materials characterized by strongly localized valence electrons and possibly, strong correlations. This activity will be fundamental to enable a reliable and quantitatively predictive use of first-principles computational techniques, e.g. on high-throughput platforms, for the identification and optimization of materials with properties very well tuned on specific technological applications.

Ab initio Computer Modeling of Materials

- Transition-metal compounds for Li-ion batteries cathodes: electronic and structural properties
- Electronic properties of transition-metal oxides (e.g., for electronics or photo-catalysis applications)
- Magneto-active and high-magnetization density alloys
- Electronic structure and excitations of molecular systems
- Structural and magnetic transitions in minerals of the Earth's interior
- Electronic and vibrational properties of correlated materials (e.g., high-T_c superconductors)
- Materials for organic and inorganic photovoltaics
- Heterogeneous catalysis in porous media
- Structural phase transformations in nanoparticles

Development of new methods and algorithms for electronic structure calculations

- Extended corrections to DFT energy functionals for strongly correlated and magnetic systems based on extended Hubbard Hamiltonians
- Self-interaction-free energy functionals and refined DFT energy spectra
- Multi-reference solution of model Hamiltonians
- Linear-response calculations of vibrational properties from Hubbard-corrected DFT functionals
- "Electronic enthalpy" functionals for finite systems under compression
- Coupled DFT – path-following-bifurcation techniques to scout new phases and transition paths in materials under external fields

Software Development

I participate to the development and maintenance of the Quantum-ESPRESSO simulation package (http://www.quantum-espresso.org). In particular, I have contributed and continue to develop corrective approaches (based on the so-called DFT+U) to perform accurate and efficient DFT calculations on correlated systems.

SCIENTIFIC PRODUCTION

Most significant accomplishments

- Introduced the DFT+U+V method, based on an additive correction to the DFT total energy modeled on the *extended* Hubbard Hamiltonian with both *on-site* (U) and *inter-site* (V) interactions. This new scheme extends the scope and improves the flexibility of the "standard" DFT+U and allows one to capture the ground state of a much broader variety of systems for which electronic localization is accompanied by a significant degree of hybridization.
- Defined a new self-interaction correction to DFT energy functionals through imposing the Koopmans condition to the Kohn-Sham spectrum. This computational scheme is able to predict the quasi-particle spectrum of isolated systems (molecules, clusters, etc) with a similar accuracy and a much lower computational cost than other methods defined for the same purpose (e.g., GW).
- Defined a linear-response approach to compute the effective Hubbard interactions (U and V) to be used in DFT+U(+V) calculations. This has become one of the reference methods to evaluate this important quantity, essential also in other corrective schemes (e.g., DFT+DMFT). The paper that first introduced it (PRB **71**, 035105 (2005)) has collected more than 1000 citations. This method has been recently

adapted to and implemented within density functional perturbation theory to greatly advance its efficiency, scalability, accuracy and user-friendliness.

- Developed an extension to density functional perturbation theory to compute vibrational spectra (and related properties) of correlated and strongly localized systems from their DFT+U ground state. This generalized algorithm will be crucial, for example, to improve the accuracy of the calculation of electron-phonon couplings and to capture finite-temperature effects in the above-mentioned materials.
- Introduced an electronic enthalpy functional for the modeling of isolated systems under static or dynamic compressions without the explicit inclusion of any pressurizing media. This functional also allows one to take into account the cavitation energy (typically modeled as a surface tension) in implicit solvation models to study systems or chemical reactions in solution.
- Identified a new phase of bulk iron (named Fe_6) with the highest known magnetization density. If stabilized at normal conditions (e.g., through doping) this phase could be the base for new technologies, including lighter, rare-earth free magnetic rotors of electrical engines and generators or higher-density information storage devices.
- Clarified the delicate relative energetics of martensite and austenite phases of Ni_2MnGa (also in dependence of Mn content) based on the interplay between magnetic and structural properties.
- Contributed to elucidate the mechanism of the spin-state crossover in $(MgFe)SiO_3$ perovskite and its implications for the behavior of the Earth's lower mantle.
- Computational characterization of electron-transfer processes between Fe ions solvated in water and first quantitative verification of the Markus theory through ab initio calculations.
- Precise quantitative characterization of the structural response of semiconductor nanoparticles to (hydrostatic and unidirectional) shock compressions and of the mechanical energy absorbed through structural deformations.
- First ab initio modeling of Li-ion battery materials with Hubbard-corrected DFT functionals showing the importance of capturing the electronic localization in the quantitative prediction of formation energies and average voltages.

RESEARCH FUNDING

Award period: 09/15 – 08/19
Title: "Nanoscience Foundries and Fine Analysis (NFFA) - Europe"
Role: co-PI (in a consortium of 20 European institutions)
Source of support: The European Commission, Horizon 2020 Framework Programme

Award period: 08/13 – 07/16
Title: "Thermoelasticity of iron-bearing minerals"
Role: Principal Investigator
Source of support: US National Science Foundation (EAR division)

Award period: July 2012 – June 2014
Title: "Efficient DFT-based computational approaches for correlated systems" (CAREER award)
Involvement: Principal Investigator
Source of support: US National Science Foundation (DMR division, CMMT program)

Award Period: 1/11/2012 – 31/10/2014
Title: "Design, modeling and synthesis of FeN nanocomposites magnet – a path to rare-earth-element free magnet for clean energy"
Involvement: co-PI
Source of support: US Department of Energy – ARPA-e

Award period: 10/09 – 09/12
Title: "Theory of thermoelastic properties of iron-bearing minerals"
Role: Principal Investigator
Source of support: US National Science Foundation (grant EAR-0810272)
Total award: $405,054
Award period: 01/09 – 12/11
Title: Abu Dhabi-Minnesota Institute for Research Excellence: ADMIRE (IRG 1.2): "Catalytic Alkane Metathesis"
Role: co-PI
Source of support: The Petroleum Institute of Abu Dhabi

TEACHING ACTIVITIES

Courses taught at the University of Pavia, 2018 – 2020

- Physics of Solid State II, master course of Physics, IV year (co-instructor)
- Fluid-dynamics and Thermodynamics, course of the bachelor degree in Physics (exercises instructor)
- Physics II, course of the bachelor degree in Chemistry (main instructor)

Courses taught at the École Polytechnique Fédérale de Lausanne (EPFL), 2013 – present

- Fundamentals of Solid-State Materials, master course of Materials Science and Engineering (exercises instructor; occasional class lectures)
- Atomistic and Quantum Simulations of Materials, master course of Materials Science and Engineering (exercises instructor; occasional class lectures)

Courses taught at the University of Minnesota, 2006 - 2013

- Mechanical Properties of Materials, core course of the graduate curriculum (main instructor; 2008 – 2012)
- Metals and Alloys, third year undergraduate course (main instructor; 2008 – 2009)
- Introduction to Materials Science and Engineering, second year undergraduate course (co-instructor; 2006 – 2007, 2011)

Teaching training

Participant of the Early Career Faculty Learning Community to Develop and Enhance Teaching Skills at the Center for Teaching and Learning of the University of Minnesota. Academic Year 2007-2008

COLLABORATORS

- Dr Iurii Timrov, Ècole polytechnique fèdèrale de Lausanne, Switzerland
- Prof. Ulrich Aschauer, University of Bern, Switzerland
- Prof. Matteo Calandra, Universitè Pierre et Marie Curie, Jussieu, France
- Dr. Daniele Passerone, EMPA, Zurich, Switzerland
- Dr. Davide Ceresoli, CNR, Milan, Italy
- Dr. G. Cherkashinin, Darmstad University, Germany

- Prof. Berend Smit, Ècole polytechnique fèdèrale de Lausanne, Switzerland
- Prof. Renata M. Mattosinho Wentzcovitch, Columbia University, New York, USA
- Prof. Andre Mkhoyan, University of Minnesota, Minneapolis, USA
- Prof. Aditya Bhan, University of Minnesota, Minneapolis, USA
- Prof. Alon McCormick, University of Minnesota, Minneapolis, USA
- Prof. Michael Tsapatsis, University of Minnesota, Minneapolis, USA
- Prof. Koichiro Umemoto, Tokyo Institute of Technology, Japan
- Prof. Andrea Floris, University of Lincoln, UK
- Dr. Burak Himmetoglu, Serimmune, Santa Barbara, USA
- Prof. Ismaila Dabo, Penn State University, USA
- Prof. Andrea Ferretti, University of Modena and Reggio Emilia, Italy
- Dr. Giovanni Borghi, University of Modena and Reggio Emilia, Italy
- Prof. Stefano de Gironcoli, International School for Advanced Studies, Italy
- Dr. Boris Kozinsky, Harvard University, Cambridge, USA

ORGANIZATION OF SCIENTIFIC MEETINGS

Co-organizer (and lecturer) of the workshop: "Advance Workshop on High-Performance & High Throughput Materials Simulations using Quantum ESPRESSO". Location: International Center for Theoretical Physics (ICTP), Trieste, Italy. Dates: 16 – 28 January 2017.

Co-organizer of the workshop: "What about U? – Effects of Hubbard Interactions and Hund's Coupling in Solids". Location: International Center for Theoretical Physics (ICTP), Trieste, Italy. Dates: 17 – 21 October 2016.

Co-organizer of a CECAM workshop, 17 – 20 June 2014, Lausanne. Title: What about U? – Strong correlation from first principles.

Co-organizer of a CECAM workshop, 18 – 21 June 2012, Lausanne. Title: What about U? - Corrective approaches to DFT for strongly-correlated systems.

Co-organizer of one session (MR03) of the AGU Fall Meeting, 2011. Title: Computational Advances and Applications in Mineral Physics

EDITORIAL ACTIVITY

Co-editor of the volume "*First Principle Approaches to Spectroscopic Properties of Complex Materials*" of the series "Topics in Current Chemistry", Springer, Volume 347 (2014)

COMMISSIONS OF TRUST

Scientific review of papers

Scientific Reports, Nano Letters, Physics Letters A, Physical Review Letters, Physical Review B, Physical Review Materials, Journal of Chemical Theory and Computation, Journal of Chemical Physics, Chemical Physics Letters, Catalysis Letters, Journal of Nanoparticle Research, Journal of the American Chemical Society, Theoretical Chemistry Accounts, Journal of Physics: Condensed Matter, Journal of Vacuum Science and Technology, Geophysical Journal International, Journal of Magnetism and Magnetic Materials, Journal of Computational Chemistry, Journal of Physical Chemistry

Grant proposal evaluation

External proposal reviewer, European Research Council Starting Grant Program, 2017
Panel reviewer, US NSF: Cyber-enabled Discovery and Innovation (CDI) program, 2011
Esternal proposal reviewer, US NSF: DMR division, 2010, 2012, 2013, 2014
External proposal reviewer, US ACS Petroleum Research Fund, 2007

INVITED TALKS AT INTERNATIONAL MEETINGS

1. M. Cococcioni, "*Ab initio modeling of transition metal compounds using the extended DFT+U+V with self-consistent Hubbard parameters*", invited presentation at the "Correlated Electron Physics beyond the Hubbard Model" CECAM – Psi-k workshop held in February 2019, in Bremen, Germany.
2. M. Cococcioni, "*First-principles modeling of transition metal compounds from Hubbard-corrected DFT functionals*", invited presentation at the Current Trends in Condensed Matter Conference, held in February 2015, at the NISER institute of Bhubaneswar, India
3. M. Cococcioni, "*Phonon dispersion of Cu oxides from ab initio DFPT+U+J calculations*", invited presentation at the American Geophysical Union annual meeting, December 2012, San Francisco, CA
4. M. Cococcioni, "*Adsorptive desulfurization of alkanes on cation-exchanged zeolites from ab initio calculations*", invited presentation at the American Chemical Society annual meeting, March 2012, San Diego, CA
5. M. Cococcioni, "*Extended LDA+U functional for covalent systems*", invited presentation at the Workshop on "Frontiers in Density Functional Theory", September 2009, Montauk, NY
6. M. Cococcioni, "*Extended LDA+U functional for covalent systems*", invited presentation at the International Materials Research Congress XVIII, August 2009, Cancun, Mexico
7. M. Cococcioni, "*Extended LDA+U functional for covalent systems*", invited presentation at the workshop ES09: 2009 Recent Development in Electronic Structure Methods, June 2009, UC Davis, CA
8. M. Cococcioni "*Ab-initio study of transition-metal compounds through a consistent, linear-response LDA+U approach*", American Geophysical Union fall meeting, December 2007, San Francisco, CA
9. M. Cococcioni "*Electronic correlation and Hubbard approaches*", invited lecture at the Quantum Simulation and Molecular Modeling workshop of the Institute for Mathematics and its Applications (IMA) of the University of Minnesota, July-August 2007, Minneapolis, MN
10. M. Cococcioni "*Nucleation and kinetics of shock-induced plastic deformations for group-IV nanoparticles from first-principles molecular dynamics*", invited presentation at the SMEC 2007 workshop, April 2007, Miami Beach, FL
11. M. Cococcioni "*A consistent, linear-response approach to LDA+U*", invited presentation at the American Physical Society March meeting, March 2006, Baltimore, MD.
12. M. Cococcioni "*Electronic-enthalpy functional for finite systems under pressure*", invited presentation at the workshop ES05 "Recent Developments in Electronic Structure Methods", June 2005, Cornell University, Ithaca, NY.
13. M. Cococcioni, G. Ceder, F. Mauri and N. Marzari, "*Thermodynamics and kinetics of group-IV nanoparticles under pressure*", invited presentation at the NIRT workshop on "Structure of nanocrystals", December 2004, Tempe AZ.

DISSEMINATION AND OUTREACH ACTIVITIES

- Lecture at the third "African School on Electronic Structure Methods and

Applications" (ASESMA2015), University of the Witwatersrand, Johannesburg, South Africa, January 18 – 31, 2015

- Lecture at the "Materials Simulations Theory and Numerics" Summer School at IISER, Pune, India, June 29 – July 12, 2014
- Lecture at the 2012 Autumn School "Correlated Electrons: From Models to Materials", Jülich, Germany, September 3 – 7, 2012
- Lecture at the 2009 Minicourse of the Mineralogy Society of America on "Theoretical And Computational Methods In Mineral Physics" (http://www.minsocam.org/MSA/SC/), UC Berkeley, CA
- Lectures at the 2009 International Center for Materials Research (ICMR) summer school at UCSB (http://media.quantum-espresso.org/santa_barbara_2009_07/index.php), Santa Barbara, CA
- Organizer and lecturer of a mini-tutorial on the "Use of DFT for Total Energy and Phonon Calculations", Department of Physics, University of Pavia, 2008
- Lectures at the Vlab tutorial at the University of Minnesota, Minneapolis, 2006 (http://www.vlab.msi.umn.edu/events/first tutorial.shtml)