Matteo Cococcioni

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CURRENT POSITION

2023 – present	Associate Professor 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 (Italian degree equivalent to B.S. + M.S.) in Physics. Department of Physics 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

2018 - 2022	Assistant Professor Physics Department, University of Pavia, Pavia, Italy
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

- More than 60 publications on peer-reviewed scientific journals or on-line archives; 3 non peer-reviewed publications (including chapters on books); 1 conference proceedings.
- Associate Professor at the Physics Department of the University of Pavia, Italy: coordination of an independent research group; teaching at both undergraduate and graduate (master) levels
- Assistant Professor at the University of Minnesota, USA: coordination of an independent research group; teaching at both undergraduate and graduate (master and PhD) levels
- Research grants 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

RESEARCH EXPERIENCE AND INTERESTS

My scientific activity focuses on the computational modeling, based on first-principles 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 dyes, catalytic systems, porous materials (e.g., zeolites and metal-organic frameworks). Besides for 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 for 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)) is very well cited. 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 the vibrational spectrum (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.

PUBLICATIONS (reverse chronological order)

1. S. Gelin, N. E. Kirchner-Hall, R. R. Katzbaer, M. J. Theibault, Y. Xiong, W. Zhao, M. M. Khan, E. Andrewlavage, P. Orbe, S. M. Baksa, M. Cococcioni, I. Timrov, Q. Campbell, H. Alruna, R. E. Schaak, I . Dabo, "*Ternary Oxides of s- and p-Block Metals for Photocatalytic Solar to Hydrogen Conversion*", Phys. Rev. X Energy **3**, 013007 (2024). https://doi.org/10.1103/PRXEnergy.3.013007.
2. I. Timrov, F. Aquilante, M. Cococcioni, N. Marzari, "*Accurate Electronic Properties and Intercalation Voltages of Olivine-Type Li-Ion Cathode Materials from Extended Hubbard Functionals*", Phys. Rev. X Energy **1**, 033003 (2022). https://doi.org/10.1103/PRXEnergy.1.033003.
3. I. Timrov, N. Marzari, M. Cococcioni, "*HP– A code for the calculation of Hubbard parameters using density-functional perturbation theory*", Comput. Phys. Comm. **279**, 108455 (2022). https://doi.org/10.24435/materialscloud:v6-zd.
4. G. Cherkashinin, R. Eilhardt, S. Nappini, M. Cococcioni, I. Pis, S. Dal Zilio, F. Bondino, N. Marwari, E. Magnano and L. Alff, "*Energy Level Alignment at the Cobalt Phosphate/Electrolyte Interface: Intrinsic Stability vs Interfacial Chemical Reactions in 5 V Lithium Ion batteries*", ACS Appl. Mater. Interfaces **14**, 543 (2022). https://doi.org/10.1021/acsami.1c16296
5. J.-J. Zhou, J. Park, I. Timrov, A. Floris, M. Cococcioni, N. Marzari, M. Bernardi, "*Ab initio Electron-Phonon Interactions in Correlated Electrons Systems*", Phys. Rev. Lett **127**, 126404 (2021). https://doi.org/10.1103/PhysRevLett.127.126404
6. M. Cappelletti, M. Leccese, M. Cococcioni, D. M. Proserpio, and R. Martinazzo, "*The Different Story of π Bonds*", Molecules **26**, 3805 (2021). https://doi.org/10.3390/molecules26133805
7. M. Cococcioni and A. Floris "*Magnetic Energy Landscape of a Dymolybdenum Tetraacetate on a Bulk Insulator Surface*", *Appl. Sci.* **11**, 3806 (2021). https://doi.org/10.3390/app11093806
8. Y. Xiong, *et al.*, "*Optimising accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen*", Energy Environ. Sci. **14**, 2335 (2021). https://10.1039/d0ee02984j
9. I. Timrov, N. Marzari, and M. Cococcioni "*Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations*", Phys. Rev. B **103**, 045141 (2021). https://doi.org/10.1103/PhysRevB.103.045141

10. I. Timrov, F. Aquilante, L. Binci, M. Cococcioni, and N. Marzari "*Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds*", Phys. Rev. B **102**, 235159 (2020). https://doi.org/10.1103/PhysRevB.102.235159
11. I. Timrov, P. Agrawal, X. Zhang, S. Erat, R. Liu, A. Braun, M. Cococcioni, M. Calandra, N. Marzari, and D. Passerone, "*Electronic structure of pristine and Ni-substituted $LaFeO_3$ from near edge x-ray absorption fine structure experiments and first-principles simulations*", Phys. Rev. Res. **2**, 033265 (2020). https://doi.org/10.1103/PhysRevResearch.2.033265
12. C. Ricca, I. Timrov, M. Cococcioni, N. Marzari and U. Aschauer, "*Self-consistent DFT+U+V study of oxygen vacancies in $SrTiO_3$*", Phys. Rev. Res. **2**, 023313 (2020). https://doi.org/10.1103/PhysRevResearch.2.023313
13. Y. Sun, M. Cococcioni, and R. M. Wentzcovitch, "*LDA+U-sc calculations of phase relations in FeO*", Phys. Rev. Mat. **4**, 063605 (2020). https://doi.org/10.1103/PhysRevMaterials.4.063605
14. A. Floris, I. Timrov, B. Himmetoglu, N. Marzari, S. de Gironcoli, and M. Cococcioni, "*Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials*", Phys. Rev. B **101**, 064305 (2020). https://doi.org/10.1103/PhysRevB.101.064305
15. M. Cococcioni and N. Marzari, "*Energetics and cathode voltages of $LiMPO_4$ olivines (M = Fe, Mn) from extended Hubbard functionals*", Phys. Rev. Mat. **3**, 033801 (2019). https://dx.doi.org/10.1103/PhysRevMaterials.3.033801
16. C. Ricca, I. Timrov, M. Cococcioni, N. Marzari and U. Aschauer, "*Self-consistent site-dependent DFT+U study of stoichiometric and defective $SrMnO_3$*", Phys. Rev. B. **99**, 094102 (2019). https://doi.org/10.1103/PhysRevB.99.094102
17. I. Timrov, N. Marzari, and M. Cococcioni, "*Hubbard parameters from density functional perturbation theory*", Phys. Rev. B **98**, 085127 (2018). https://link.aps.org/doi/10.1103/PhysRevB.98.085127
18. P. Giannozzi, et al., "*Advanced capabilities for materials modelling with Quantum ESPRESSO*", Journal of Physics: Condensed Matter **29**, 465901 (2017). https://doi.org/10.1088/1361-648X/aa8f79
19. M. L. Odlyzko, B. Himmetoglu, M. Cococcioni, and K. A. Mkhoyan, "*Atomic bonding effects in annular dark field scanning transmission electron microscopy. I. Computational predictions*", Journal of Vacuum Science and Technology A **34**, 041603 (2016). http://dx.doi.org/10.1116/1.4954871
20. G. Shukla, M. Cococcioni, and R. M. Wentzcovitch, "*Thermoelasticity of Fe^{3+} and Al-bearing bridgmanite*", Geophysical Research Letters **43**, 5661 (2016) http://dx.doi.org/10.1002/2016GL069332
21. G. W. Mann, K. Lee, M. Cococcioni, B. Smit, J. B. Neaton, "*First-Principles Hubbard U Approach for Small Molecule Binding in Metal-Organic Frameworks*", the Journal of Chemical Physics **144**, 174104 (2016) http://dx.doi.org/10.1063/1.4947240.
22. Y. Jiang, B. Himmetoglu, M. Cococcioni, and J.-P. Wang, "*DFT calculation and experimental investigation of Mn doping effects in $Fe_{16}N_2$*", AIP Advances **6**, 056007 (2016) http://dx.doi.org/10.1063/1.4943059
23. G. Shukla, Z. Wu, H. Hsu, A. Floris, M. Cococcioni, and R. M. Wentzcovitch, "*Thermoelasticity of Fe^{2+}-bearing bridgmanite*", Geophysical Research Letters **42**, 1741 (2015) http://dx.doi.org/10.1002/2014GL062888.
24. K. Umemoto, B. Himmetoglu, J.-P. Wang, Renata M. Wentzcovitch, and M. Cococcioni, "*Searching for high magnetization density in Fe: The new metastable Fe_6 phase*", Journal of Physics: Condensed Matter **27**, 016001 (2015) http://dx.doi.org/10.1088/0953-8984/27/1/016001.
25. A. Ferretti, I. Dabo, M. Cococcioni, and N. Marzari, "*Bridging density functional and many-body perturbation theory: orbital-dependence in electronic-structure functionals*", Physical Review B **89**, 195134 (2014) http://dx.doi.org/10.1103/PhysRevB.89.195134.
26. B. Himmetoglu, A. Floris, S. de Gironcoli, and M. Cococcioni, "*Hubbard-corrected DFT functionals: the LDA+U description of correlated systems*", (invited review article) International Journal of Quantum Chemistry **114**, 14-49 (2014) http://dx.doi.org/10.1002/qua.24521.

27. M. Mazar, S. Al Hashimi, M. Cococcioni and A. Bhan, "*b-scission of Olefins on Acidic Zeolites: A Periodic PBE-D Study in H-ZSM-5*", Journal of Physical Chemistry C **117**, 23609 (2013) http://dx.doi.org/10.1021/jp403504n.
28. C.-Y. Sung, S. Al Hashimi, A. McCormick, M. Cococcioni, M. Tsapatsis, "*A DFT study on multivalent cation-exchanged Y zeolites as potential selective adsorbent for H_2S*", Microporous and Mesoporous Materials **172**, 7-12 (2013). http://dx.doi.org/10.1016/j.micromeso.2012.12.006
29. I. Dabo, A. Ferretti, C.-H. Park, N. Poilvert, Y. Li, M. Cococcioni, and N. Marzari, "*Donor and acceptor levels of organic photovoltaic compounds from first principles*", Physical Chemistry Chemical Physics **15**, 685-695 (2013). http://dx.doi.org/10.1039/C2CP43491A
30. B. Himmetoglu, A. Marchenko, I. Dabo, and M. Cococcioni, "*Role of electronic localization in the phosphorescence of iridium sensitizing dyes*", Journal of Chemical Physics **137**, 154309 (2012). http://dx.doi.org/10.1063/1.4757286
31. M. Mazar, S. Al Hashimi, A. Bhan, M. Cococcioni, "*The Methylation of Ethene by Surface Methoxides: A Periodic PBE+D Study across Zeolites*", Journal of Physical Chemistry C **116**, 19385 (2012). http://dx.doi.org/10.1021/jp306003e
32. A. Khare, B. Himmetoglu, M. Cococcioni, E. Aydil, "*First principles calculation of the electronic properties and lattice dynamics of $Cu_2ZnSn(S_{1-x}Se_x)_4$*", Journal of Applied Physics **111**, 123704 (2012). http://dx.doi.org/10.1063/1.4728232
33. B. Himmetoglu, V. M. Katukuri, and M. Cococcioni, "*Origin of magnetic interactions and their influence on the structural properties of Ni_2MnGa and related compounds*", Journal of Physics: Condensed Matter **24**, 185501 (2012). http://dx.doi.org/10.1088/0953-8984/24/18/185501.[1]
34. Y. Yu, H. Hsu, M. Cococcioni, and R. M. Wentzcovitch, "*Spin state and hyperfine interactions of iron incorporated in $MgSiO_3$*", Earth and Planetary Science Letters **331 – 332**, 1 (2012). http://dx.doi.org/10.1016/j.epsl.2012.03.002
35. A. Khare, B. Himmetoglu, M. Johnson, D. J. Norris, M. Cococcioni, and E. S. Aydil, "*Calculation of the lattice dynamics and Raman spectra of copper zinc tin chalcogenides and comparison to experiments*", Journal of Applied Physics **111**, 083707 (2012). http://dx.doi.org/10.1063/1.4704191
36. C.-Y. Sung, S. Al Hashimi, A. McCormick, M. Tsapatsis, and M. Cococcioni, "*A DFT study on the adsorption of H_2S and other Claus process tail gas components on Cu- and Ag-exchanged Y zeolites*", Journal of Physical Chemistry C **116**, 3561 – 3575 (2012). https://dx.doi.org/10.1021/jp2097313
37. A. Floris, S. de Gironcoli, E. K. U. Gross, and M. Cococcioni, "*Vibrational Properties of MnO and NiO from DFT+U-based Density Functional Perturbation Theory*", Physical Review B **84**, 161102(R) (2011). http://dx.doi.org/10.1103/PhysRevB.84.161102.[2]
38. D. B. Ghosh, M. Cococcioni, and R. S. Elliott, "*Structural phase transition path-following and stable phase scouting through a coupled DFT-BFB algorithm*", Modeling and Simulation in Materials Science and Engineering **19**, 085007 (2011). http://dx.doi.org/10.1088/0965-0393/19/8/085007.
39. K. Varoon, X. Zhang, B. Elyassi, D. Brewer, M. Gettel, S. Kumar, J. A. Lee, S. Maheshwari, A. Mittal, C.-Y. Sung, M. Cococcioni, L. F. Francis, A. V. McCormick, A. Mkhoyan, and M. Tsapatsis, "*Dispersible Exfoliated Zeolite Nanosheets and Their Application as a Selective Membrane*", Science **334**, 72 (2011). http://dx.doi.org/10.1126/science.1208891.
40. P. Kumar, C.-Y. Sung, O. Muraza, M. Cococcioni, S. Al Hashimi, A. McCormick, and M. Tsapatsis, "*H_2S adsorption by Ag and Cu Ion-Exchanged Faujasites*", Microporous and Mesoporous Materials **146**, 127-133 (2011). http://dx.doi.org/10.1016/j.micromeso.2011.05.014.

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[1] This work was highlighted as a cover-story of the journal: "*New insights on martensitic transitions in Ni-Mn-Ga alloys*".

[2] The paper was selected as an "Editor's suggestion".

41. B. Himmetoglu, R. M. Wentzcovitch, and M. Cococcioni, "*First principles study of the electronic and structural properties of CuO*", Physical Review B **84**, 115108 (2011). http://dx.doi.org/10.1103/PhysRevB.84.115108.
42. M. Mazar, S. Al Hashimi, A. Bhan, and M. Cococcioni, "*Alkane Metathesis by Tantalum Metal Hydride of Ferrierite: A Computational Study*", J. Phys. Chem. C **115** (20), 10087-10096 (2011). http://dx.doi.org/10.1021/jp200756e.
43. H. Hsu, P. Blaha, M. Cococcioni, and R. M. Wentzcovitch, "*Spin-state crossover and hyperfine interactions of ferric iron in (Mg,Fe)SiO_3 perovskite*", Phys. Rev. Lett. **106**, 118501 (2011). http://dx.doi.org/10.1103/PhysRevLett.106.118501.[3]
44. H. Hsu, K. Umemoto, M. Cococcioni, and R. M. Wentzcovitch, "*The Hubbard U correction for iron-bearing minerals: A discussion based on (Mg,Fe)SiO_3 perovskite*", Phys. Earth Planet. In. **185**, 13-19 (2011), http://dx.doi.org/10.1016/j.pepi.2010.12.001.
45. I. Dabo, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, "*Koopmans' condition for density-functional theory*", Phys. Rev. B **82**, 115121 (2010). http://dx.doi.org/10.1103/PhysRevB.82.115121.
46. V. L. Campo Jr. and M. Cococcioni, "*Extended DFT+U+V method with on-site and inter-site electronic interactions*", J. Phys.: Condens. Matter **22**, 055602 (2010). http://dx.doi.org/10.1088/0953-8984/22/5/055602.[4]
47. P. Giannozzi, et al., "*Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials*", J. Phys.: Condens. Matter **21**, 395502 (2009). http://dx.doi.org/10.1088/0953-8984/21/39/395502.
48. H. Hsu, K. Umemoto, M. Cococcioni, R. M. Wentzcovitch, "*First-principles study for low-spin $LaCoO_3$ with a structurally consistent Hubbard U*", Phys. Rev. B **12**, 125124 (2009). http://dx.doi.org/10.1103/PhysRevB.79.125124.
49. H.-L. Sit, M. Cococcioni, and N. Marzari, "*Car-Parrinello molecular dynamics in the DFT+U formalism: Structure and energetics of solvated ferrous and ferric ions*", Journal of Electroanalytical Chemistry **607**, 107 - 112 (2007). http://dx.doi.org/10.1016/j.jelechem.2007.01.008.
50. D. A. Scherlis, M. Cococcioni, H.-L. Sit and N. Marzari, "*Simulation of Heme using DFT+U: a step toward accurate spin-state energetics*", Journ. of Phys. Chem B **111**, 7384-7391 (2007). http://dx.doi.org/10.1021/jp070549l.
51. H. J. Kulik, M. Cococcioni, and N. Marzari, "*Density functional theory in transition-metal chemistry: a self-consistent Hubbard U approach*", Phys. Rev. Lett. **97**, 103001 (2006). http://dx.doi.org/10.1103/PhysRevLett.97.103001.
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54. M. Cococcioni, F. Mauri, G. Ceder and N. Marzari, "*Electronic-enthalpy functional for finite systems under pressure*", Phys. Rev. Lett. **94**, 145501 (2005). http://dx.doi.org/10.1103/PhysRevLett.94.145501.
55. M. Cococcioni and Stefano de Gironcoli, "*Linear response approach to the calculation of the effective interaction parameters in the LDA+U method*", Phys. Rev. B. **71**, 035105 (2005). http://dx.doi.org/10.1103/PhysRevB.71.035105.
56. F. Zhou, M. Cococcioni, A. C. Marianetti, D. Morgan and G. Ceder, "*First-principles prediction of redox potentials in transition-metal compounds with LDA+U*", Phys. Rev. B. **70**, 235121 (2004). http://dx.doi.org/10.1103/PhysRevB.70.235121.

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[3] This article was featured on the cover of Phys. Rev. Lett., March 18th 2011. The work was also highlighted in the Physics Today magazine, May 2011 issue.

[4] The topic of the paper was highlighted in the cover-story of the journal: "*Mott insulators on the verge of a localization crisis*" http://iopscience.iop.org/0953-8984/labtalk-article/41854. This article was also selected for the Highlight of 2010 selection of the journal: http://iopscience.iop.org/0953-8984/page/Highlights of 2010.

57. F. Zhou, M. Cococcioni, K. Kang and G. Ceder, "*The Li intercalation potential of $LiMPO_4$ and $LiSiO_4$ olivines with M = Fe, Mn, Co, Ni*", Electrochemistry Communications **6**, 1144 (2004). http://dx.doi.org/10.1016/j.elecom.2004.09.007.
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59. R. M. Wentzcovitch, B. B. Karki, M. Cococcioni and S. de Gironcoli, "*Thermoelastic properties of $MgSiO_3$-Perovskite: insight on the nature of the Earth's lower mantle*", Phys. Rev. Lett. **92**, 18501 (2004). http://dx.doi.org/10.1103/PhysRevLett.92.018501.[5]
60. M. Cococcioni, A. Dal Corso and S. de Gironcoli, "*Structural, electronic, and magnetic properties of Fe_2SiO_3 fayalite: comparison of LDA and GGA results*", Phys. Rev. B **67**, 094106 (2003). http://dx.doi.org/10.1103/PhysRevB.67.094106.
61. M. Cococcioni and M. Acquarone, "*A non-perturbative treatment of the generalized Su-Shrieffer-Heeger Hamiltonian on a dimer*", Int. J. of Mod. Phys. B **14** n. 25-27, 2956 (2000). http://dx.doi.org/10.1142/S0217979200003162.

Non-refereed Papers and Book Chapters

1. I. Dabo, A. Ferretti, G. Borghi, N. L. Nguyen, N. Poilvert, C-H Park, M. Cococcioni, N. Marzari, "*Piecewise linearity and spectroscopic properties from Koopmans-compliant functionals*", October 2013 Psi-k Scientific Highlight article (Newsletter 119).
2. M. Cococcioni, "*The LDA+U Approach: A Simple Hubbard Correction for Correlated Ground States*", Chapter in the book: CORRELATED ELECTRONS: FROM MODELS TO MATERIALS, Lecture Notes of the Autumn School Correlated Electrons 2012 (Jülich, September 3 – 7, 2012), E. Pavarini, E. Koch, F. Anders, and M. Jarrell editors. http://hdl.handle.net/2128/4611.
3. M. Cococcioni, "*Accurate and Efficient Calculations on Strongly Correlated Minerals with the LDA plus U Method: Review and Perspectives* ", THEORETICAL AND COMPUTATIONAL METHODS IN MINERAL PHYSICS: GEOPHYSICAL APPLICATIONS Book Series: Reviews in Mineralogy & Geochemistry **71**, 147-167 (2010), R. M. Wentzcovitch, and L. Stixrude, editors. http://dx.doi.org/10.2138/rmg.2010.71.8.

Conference Proceedings

1. D. B. Ghosh, M. Cococcioni, and R. S. Elliott, "*Structural phase transition path-following and stable phase scouting through a coupled DFT-BFB algorithm*", Proceedings of SPIE volume 7647, article number UNSP 76474P (2010), Conference on Sensors and Smart Structures Technologies for Civil, Mechanical, and Aerospace Systems 2010

ARTICLES IN PREPARATION

1. M. Cococcioni and N. Marzari, "*Deformation mechanisms of group-IV nanoparticles under hydrostatic shock compression from first-principles*"

HONORS AND AWARDS

Funding

US National Science Foundation CAREER award ($410,000) from the CMMT program in the DMR division, December 2011.

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[5] The study presented in this article was also selected for the Phys. Rev. Focus "*What's down there?*", (2004).

Visiting Scholar Positions

Junior Researcher Funded Visit from the London Thomas Young Centre for Theory and Simulations of Materials, King's College (Department of Physics), London, July 2010. Focus of the visit: Development of DFT-based computational approaches for correlated materials.

Other recognitions

UIUC Physical Chemistry Student Selected Speaker, Department of Chemistry, University of Illinois at Urbana Champaign. Presentation title: "*From the Koopmans theorem to the electronic correlation: how well can we do with DFT?*", April 2010.

Invited presentations 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 CCP2022 IUPAP Conference on Computational Physics, August 2022, Austin, Texas, USA
2. M. Cococcioni, "*Ab initio modeling of transition metal compounds using the extended DFT+U+V with self-consistent Hubbard parameters*", invited presentation at the COSMIC "Magnetic Molecule on Surface" virtual workshop, March 2021, Paris, France
3. 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.
4. 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
5. 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
6. 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
7. M. Cococcioni, "*Extended LDA+U functional for covalent systems",* invited presentation at the Workshop on "Frontiers in Density Functional Theory", September 2009, Montauk, NY
8. M. Cococcioni, "*Extended LDA+U functional for covalent systems*", invited presentation at the International Materials Research Congress XVIII, August 2009, Cancun, Mexico
9. 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
10. 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
11. 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
12. 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
13. M. Cococcioni "*A consistent, linear-response approach to LDA+U*", invited presentation at the American Physical Society March meeting, March 2006, Baltimore, MD.

14. 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.
15. 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.

RESEARCH FUNDING

Award period: 09/23 - 08/25
Title: "Xiss: Chirality Induced Spin Selectivity"
Role: Principal Investigator
Source of support: The Italian Ministry of University and Research
Total award: € 189,976

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
Total award: € 3,248,329.00

Award period: 08/13 – 07/16
Title: "Thermoelasticity of iron-bearing minerals"
Role: Principal Investigator
Source of support: US National Science Foundation (EAR division)
Total award: $366,000

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)
Total award: $410,000

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
Total award: $3,044,103

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
Total award: $745,608

TEACHING ACTIVITIES

Courses taught at the University of Pavia, 2018 – 2020

- Solid State Physics II, master course in Physics (main instructor)
- Fluids 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 – 2018

- 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

SUPERVISION AND MENTORING

Post-doctoral research associates

- Dr Maria Barbara Maccioni. Period: 2022 - present. Topics: ring-shaped magnetic nanomagnets for Quantum Science and Technology applications
- Dr Burak Himmetoglu. Period: 2010 – 2012. Topics: Ir dyes, magnetic shape-memory and high-magnetization density alloys, transition-metal oxides, mantle's minerals, method development. Current position: Senior Manager of Data Science at Optum, USA.
- Dr Chun-Yi Sung. Period: 2009 – 2012 (co-advised with Michael Tsapatsis and Alon McCormick). Topics: catalytic hydrocarbon purification in activated porous materials. Present position: Research Associate at the Department of Chemical Engineering of Northwestern University.
- Dr Dipta Bhanu Ghosh. Period: 2008 – 2010. (co-advised with Ryan S. Elliott, AEM). Topics: Coupled DFT – bifurcation numerical techniques to study phase transformation pathways in solids. Present position: Research Scientist, Louisiana State University
- Dr Vivaldo Leiria Campo Jr. Period: 2007 – 2008. Topics: development of the extended DFT+U+V functional. Present position: Associate Professor, Department of Physics, Federal University of Sao Carlos, Brazil.

- Dr Prasanjit Samal. Period: 2007 – 2008. Topics: development of a generalized electronic enthalpy functional for the uniaxial compression of isolated systems. Present position: Assistant Professor, School of Physical Science, NISER, P. O. Sainik School, Orissa, India

Graduate (Ph.D and Master) Students

Master's Theses Directed

- Lorenzo Marti (University of Pavia). Period: 2022 - 2023 academic year. Topic: synthesis, characterisation and computational modelling of transition-metal fluorophosphates as prospect cathode materials for Na-ion batteries.
- Elia Stocco (University of Pavia). Period: 2021 - 2022 academic year. Topic/title of the thesis: "DFT study of octonuclear molecular nano-magnets", June 2022.
- Vamshi Mohan Katukuri (University of Minnesota). Period: 2009 – 2011. Topics: martensitic transformations in Ni-Mn-Ga alloys. Master thesis: "A DFT+U Study of a Ni-Mn-Ga Magnetic Shape Memory Alloy", March 2011.

Doctoral Students Advised

- Lorenzo Marti (University of Pavia). Period: 2023 - present. Topics: joint computational and experimental study of materials for Na- and F-ion batteries.
- Mark N. Mazar (University of Minnesota). Period: 2007 – 2013. Topics: hydrocarbon chemistry in porous media. Ph.D Thesis: "First Principles Simulations of Hydrocarbon Conversion Processes in Functionalized Zeolites", May 2013.
- Gaurav Shukla (University of Minnesota). Period: 2011 – 2016 (co-advised with R. M. Wentzcovitch). Topics: thermo-elastic properties of transition-metal minerals in the Earth's mantle. Thesis: "Thermoelastic Properties of iron- and aluminum-bearing bridgmanite at high pressures and temperatures", January 2016.

Undergraduate Students

- Matteo Piras, bachelor student (University of Pavia). Period: 2020 - 2021 academic year. Topic/title of the thesis: "Resonance, aromaticity and electronic delocalisation from the resonance bond theory", July 2021.
- Zachary Zadow (University of Minnesota). Period: summer term of 2011. Topic: electronic properties of Cu_2O.
- Alex Marchenko (University of Minnesota). Period: spring - summer terms of 2010. Topics: electronic excitations in selected Ir-centered phosphorescent dyes used for organic photovoltaics. A paper resulted from his work: Journal of Chemical Physics **137**, 154309 (2012). After his research experience in my group, Alex Marchenko was then accepted in the European Master Program MaNuEn (http://phelma.grenoble-inp.fr/courses/master-manuen-materials-science-for-nuclear-energy-280251.kjsp). Alex Marchenko was awarded 2nd place at the AIChE Student Paper Competition at Michigan Tech (Houghton, MI) in April 2011, presenting his UROP project, developed under my supervision.

COLLABORATORS

- Prof. Rocco Martinazzo, University of Milan, Italy

- 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 Advanced Quantum ESPRESSO Tutorial: "Hubbard and Kopmans Functionals From Linear Response". Location: University of Pavia, Italy. Dates: 28 August - 1 September 2023

Co-organizer (and lecturer) of the Advanced Quantum ESPRESSO (online) Tutorial: "Hubbard and Kopmans Functionals From Linear Response". Dates: 9 - 11 November 2022

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 Special Issue "*Modeling Transition-Metal Systems: Emerging Developments and Applications*" of the Applied Sciences magazine, 2021

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

Nature Communications, Scientific Reports, Journal of Applied Physics, Nano Letters, Journal of Physical Chemistry Letters, Physics Letters A, Physical Review Letters, Physical Review B, Physical Review Materials, Computational Materials Science, 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, Chilean National Research and Development Agency, 2022
External proposal reviewer, US National Science Foundation Career Program, 2021
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

SCIENTIFIC SOCIETIES

Swiss Physical Society (2014 – 2018), American Physical Society (2004 – 2013), American Geophysical Union (2007 – 2012), American Chemical Society (2012)

ASSOCIATIONS

Alumnus of the Collegio Ghislieri of Pavia. Residency at the Collegio, during undergraduate Physics studies (1994-1999)

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)

INVITED SEMINARS

1. M. Cococcioni, "*Ab initio modeling of Li-ion batteries cathodes: from the Nobel Prize to open challenges*", invited seminar at the International School for Advanced Studies (SISSA), October 2019, Trieste, Italy.
2. M. Cococcioni, "*Modeling transition-metal compounds from extended Hubbard functionals*", invited seminar at the Physics department of the University of Pavia, May 2018, Pavia, Italy.
3. M. Cococcioni, "*Transition-metal compounds from extended Hubbard functionals*", invited seminar at the Physics department of the State University of Milan, April 2018, Milan, Italy.
4. M. Cococcioni, "*Modellizzazione ab initio di composti di metalli di transizione*", invited seminar at the Physics department of the University of Rome La Sapienza, December 2016, Rome, Italy.
5. M. Cococcioni, "*First-principles modeling of transition metal compounds from Hubbard-corrected DFT functionals*", invited seminar at the Max Planck Institute for Solid State Research, March 2015, Stuttgart, Germany.
6. M. Cococcioni, "Ab initio modeling of transition metal compounds with Hubbard-corrected DFT functionals", invited department seminar at the Jülich Forschungszentrum, November 2014, Jülich, Germany
7. M. Cococcioni, "*Corrections to exchange-correlation functionals for correlated systems: DFT+U*", invited lecture at the Materials Simulations Theory and Numerics summer school, Indian Institute of Science, Education and Research (IISER), July 2014, Pune, India
8. M. Cococcioni, "*Modeling strongly correlated systems with Hubbard-corrected DFT functionals*", Niels Bohr Institute, University of Copenhagen, September 2013, Copenhagen, Denmark
9. M. Cococcioni, "*Accurate materials modeling from extended DFT functionals*", School of Physics, Trinity College, May 2013, Dublin, Ireland
10. M. Cococcioni, "*Accurate materials modeling from extended DFT functionals*", School of Physics and Astronomy, University of Edinburgh, December 2012, Edinburgh, UK
11. M. Cococcioni, "*Accurate and efficient modeling of correlated systems with Hubbard-corrected DFT*", Department of Physics, November 2012, University of Durham, Durham, UK
12. M. Cococcioni, "*Accurate modeling of transition-metal-based materials with Hubbard-corrected DFT*", Department of Physics, September 2012, Queen's University, Belfast, UK
13. M. Cococcioni, "*The LDA+U Approach: A Simple Hubbard Correction for Correlated Ground States*", invited lecture at the Correlated Electrons 2012 Autumn School, September 2012, Jülich, Germany
14. M. Cococcioni, "*Accurate and predictive modeling of transition-metal-based materials and their applications*", invited presentation at the Robert Bosch Research and Technology Center, July 2012, Palo Alto, CA
15. M. Cococcioni, "*Accurate and predictive modeling of transition-metal compounds and their applications*", invited seminar at the Department of Physics, King's College, March 2012, London
16. M. Cococcioni, "*Electronic localization and magnetism in transition metal compounds from ab initio calculations*", invited lecture of the Magnetic Seminars series, Department of Electrical and Computer Engineering, University of Minnesota, February 2012, Minneapolis, MN
17. M. Cococcioni, "*A unified treatment of band and Mott insulators from the extended Hubbard model*", Materials Modeling Laboratory Seminar, Department of Materials, University of Oxford, October 2010, Oxford
18. M. Cococcioni, "*Ab-initio Hubbard-model corrections for DFT functionals*", Thomas Young Centre Soiree, Department of Physics, King's College, July 2010, London
19. M. Cococcioni, "*From the Koopmans theorem to the electronic correlation: how well*

can we do with DFT?", Department of Chemistry, University of Urbana Champaign, April 2010, Urbana, IL

20. M. Cococcioni, "*Advances in the LDA+U method for strongly correlated materials*", short course on "*Theoretical And Computational Methods In Mineral Physics: Applications To Geophysics*", UC Berkeley, December 2009, Berkeley, CA
21. M. Cococcioni, "*First-principles DFT+U in the PWscf code*" and "*Magnetism and correlation in open-shell systems*", lectures at the ICMR summer school on Materials Modeling from First Principles: Theory and Practice, UCSB, July 2009, Santa Barbara, CA
22. M. Cococcioni, "*First-Principles LDA+U+V for covalent systems*", invited seminar at the Department of Materials Science, Università di Milano-Bicocca, June 2009, Milan, Italy
23. M. Cococcioni, "*Pressure-induced transformations in semiconductor nanoparticles*" invited seminar, Department of Physics, Ohio State University, November 2008, Columbus, OH
24. M. Cococcioni, tutorial on: "*First-principles DFT+U in the PWscf code*", Vlab tutorial at UCSB, July 2008, Santa Barbara, CA
25. M. Cococcioni, invited seminar and tutorial on: "*Plane-wave, pseudopotential implementation of Density-Functional Theory for total energy and phonon calculations*", Department of Physics, University of Pavia, May 2008, Pavia, Italy
26. M. Cococcioni "*Improved numerical methods for transition-metal compounds*", invited seminar at the Department of Physics, Condensed Matter Sector, University of Minnesota, October 2007, Minneapolis, MN
27. M. Cococcioni "*Nucleation and kinetics of shock-induced plastic deformations for group-IV nanoparticles from first-principles molecular dynamics*", invited seminar at the Department of Aerospace and Mechanics, University of Minnesota, February 2007, Minneapolis, MN
28. M. Cococcioni "*Nucleation and kinetics of shock-induced plastic deformations for group-IV nanoparticles from first-principles molecular dynamics*", invited seminar at the Nanoparticle Science and Engineering Seminar Series, University of Minnesota, February 2007, Minneapolis, MN.
29. M. Cococcioni "*Plasticity and energy absorption at the nanoscales: kinetics and chemical control*", invited seminar at Yeshiva University, April 2006, New York City, NY.
30. M. Cococcioni "*Engineering the electronic and structural properties of advanced materials with first-principles calculations", invited seminar at the* Dapartment of Chemical Engineering and Materials Science, University of Minnesota, May 2005, Minneapolis, MN.
31. M. Cococcioni, N. Marzari, "*Electronic-enthalpy functional for first-principles molecular dynamics of finite systems under pressure*", invited seminar at the University of Modena, July 2004, Modena, Italy.
32. M. Cococcioni, F. Mauri, G. Ceder and N. Marzari, "*Designing new materials with ab-initio calculations*", invited seminar at the Condensed Matter Sector of the International School for Advanced Studies (SISSA - ISAS), May 2004, Trieste, Italy.
33. M. Cococcioni, G. Ceder, N. Marzari, "*Structure and dynamics of semiconductor nanoparticles under shock wave*", invited seminar at the Physics department of the University of Pavia, December 2003, Pavia, Italy.