PUBLICATIONS

1. Iurii Timrov, Nicola Marzari, and Matteo Cococcioni *"Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations"*, arXiv:2011.03271, to appear on Phys. Rev. B (2021)
2. Iurii Timrov, Francesco Aquilante, Luca Binci, Matteo Cococcioni, and Nicola 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
3. Iurii Timrov, Piyush Agrawal, Xinyu Zhang, Selma Erat, Riping Liu, Artur Braun, Matteo Cococcioni, Matteo Calandra, Nicola Marzari, and Daniele 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
4. C. Ricca, I. Timrov, M. Cococcioni, N. Marzari and U. Aschauer, *"Self-consistent DFT+U+V study of oxygen vacancies in $SrTiO_3$"*, Phys. Res. B. **2**, 023313 (2020). https://doi.org/10.1103/PhysRevResearch.2.023313
5. 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
6. 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
7. 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
8. 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
9. 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
10. 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
11. 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
12. 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.
13. 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.
14. 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

15. 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.
16. 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.
17. 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.
18. 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.
19. 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.
20. 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
21. 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
22. 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
23. 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
24. 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
25. 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]
26. 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
27. 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
28. 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*

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

Ag-exchanged Y zeolites", Journal of Physical Chemistry C **116**, 3561 – 3575 (2012). http://dx.doi.org/10.1021/jp2097313

29. 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]
30. 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.
31. 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.
32. 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.
33. 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.
34. 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.
35. 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]
36. 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.
37. 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.
38. 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]
39. 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.
40. 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.
41. 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

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

of Electroanalytical Chemistry **607**, 107 - 112 (2007). http://dx.doi.org/10.1016/j.jelechem.2007.01.008.

42. 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.
43. 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.
44. H.-L. Sit, M. Cococcioni, and N. Marzari, *"Realistic, quantitative descriptions of electron-transfer reactions: diabatic surfaces from first-principles molecular dynamics",* Phys. Rev. Lett. **97**, 028303 (2006). http://dx.doi.org/10.1103/PhysRevLett.97.028303.
45. D. Scherlis, J.-L. Fattebert, F. Gygi, M. Cococcioni, and N. Marzari, *"A unified electrostatic and cavitation model for first-principles molecular dynamics in solution",* J. Chem. Phys. **124**, 074103 (2006). http://dx.doi.org/10.1063/1.2168456.
46. 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.
47. 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.
48. 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.
49. 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.
50. F. Zhou, A. C. Marianetti, M. Cococcioni, D. Morgan and G. Ceder, *"Phase separation in Li_xFePO_4 induced by correlation effects",* Phys. Rev. B. **69**, 201101 (2004). http://dx.doi.org/10.1103/PhysRevB.69.201101.
51. 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]
52. 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.
53. 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

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

(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