Chris A. Marianetti

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and Applied Physics and Applied Mathematics
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Education

Ph.D. 2004, Massachusetts Institute of Technology, Mat. Sci. and Eng.
M.S. 1998, The Ohio State University, Welding Engineering
B.S. 1997, The Ohio State University, Welding Engineering

Experience

Assoc. Prof., Dept. of App. Physics and App. Math, Columbia Univ., July 2013-Present
Asst. Prof., Dept. of App. Physics and App. Math, Columbia Univ., July 2008-June 2013
Postdoctoral Researcher, Lawrence Livermore National Laboratory, July 2007-July 2008
Postdoctoral Researcher, Rutgers University, Feb 2004-June 2007

Research Interests

Density functional theory, Dynamical mean-field theory, energy generation/storage materials, strongly correlated electrons, Phonon interactions, actinides, transition-metal oxides, monolayer materials.

Major Awards

NSF Career Award, DARPA Young Faculty Award

Current PhD Students

Eric Isaacs, Xinyuan Ai (Physics), Chanul Kim, Mordechai Kornbluth, Chengzheng Qian.

Current Postdocs

Hyowon Park, Yue Chen, Pierre Darancet, Jia Chen, and Dalal Kanan.

Journal Referee

Physical Review B, Physical Review Letters, Proceedings of the Royal Society, Acta Crystallographica, Solid State Communications, Journal of Chemical Theory and Computation, European Physics Letters, New Journal of Physics, Acta Materialia.

Review Panels

NSF, Los Alamos LDRD Review, Army Research Laboratory Review Panel.

Professional Societies

American Physical Society, Materials Research Society.

Editor

Emerging areas of actinide science
MRS Bull., Vol. 35, No. 11 (November 2010) pp. 825-936

Publications: H-Index=21, Total Citations=2751 [Google Scholar 4/6/2015]

1. *Density Functional plus Dynamical Mean-Field Theory of the Spin-Crossover Molecule $Fe(phen)_2(NCS)_2$*
   J. Chen, A.J. Millis, and C.A. Marianetti
   arXiv:1503.03547 (2015)

2. *Origin of Spinel Nanocheckerboards via First Principles*
   M. Kornbluth and C.A. Marianetti
   arXiv:1501.03480 (2015)

3. *Charge transfer across transition metal oxide interfaces: emergent conductance and new electronic structure*
   H. Chen, H. Park, A.J. Millis, and C.A. Marianetti
   Phys. Rev. B 90, 245138 (2014)

4. *Computing total energies in complex materials using charge self-consistent DFT+DMFT*
   H. Park, A.J. Millis, and C.A. Marianetti
   Phys. Rev. B 90, 235103 (2014)

5. *Selectively Localized Wannier Functions*
   R. Wang, E.A. Lazar, H. Park, A.J. Millis, and C.A. Marianetti
   Phys. Rev. B 90, 165125 (2014)

6. *Density functional plus dynamical mean field theory of the metal-insulator transition in early transition metal oxides*
   H.T. Dang, X. Ai, A.J. Millis, and C.A. Marianetti
   Phys. Rev. B 90, 125114 (2014)

7. *First-principles approach to nonlinear lattice dynamics: Anomalous spectra in PbTe*
   Y. Chen, X. Ai, and C.A. Marianetti
   Phys. Rev. Lett. 113, 105501 (2014)

8. *A slave mode expansion for obtaining ab-initio interatomic potentials*
   X. Ai, Y. Chen, and C.A. Marianetti
   Phys. Rev. B 90, 014308 (2014)

9. *Three-dimensional metallic and two-dimensional insulating behavior in octahedral tantalum dichalcogenides*
   P. Darancet, A.J. Millis, C.A. Marianetti
   Phys. Rev. B 90, 045134 (2014)

10. *Total energy calculations using DFT+DMFT: computing the pressure phase diagram of the rare earth nickelates*
    H. Park, A.J. Millis, C.A. Marianetti
    Phys. Rev. B 89, 245133 (2014)

11. *Ideal strength and phonon instability of strained monolayer materials*
    E.B. Isaacs and C.A. Marianetti
    Phys. Rev. B 89, 184111 (2014)

12. *The failure of DFT computations for a stepped-substrate-supported monatomic highly-correlated wire system*
N. Zaki, H. Park, R.M. Osgood, A.J. Millis, and C.A. Marianetti
Phys. Rev. B 89, 205427 (2014)

13. *Covalency and the metal-insulator transition in titanate and vanadate perovskites*
H.T. Dang, A.J. Millis, and C.A. Marianetti
Phys. Rev. B 89, 161113 (2014)

14. *Physical adsorption and Charge Transfer of molecular Br2 on Graphene*
Z. Chen, P. Darancet, L. Wang, A.C. Crowther, C.R. Dean, T. Taniguchi, K. Watanabe, J. Hone, C.A. Marianetti, and L.E. Brus
ACS Nano 8 , 2943 (2014)

15. *Correlation and relativistic effects in U metal and U-Zr alloy: Validation of ab initio approaches*
W. Xie, W. Xiong, C.A. Marianetti, and D.D. Morgan
Phys. Rev. B 88, 235128 (2013)

16. *Engineering Correlation Effects via Artificially Designed Oxide Superlattices*
H. Chen, A.J. Millis, and C.A. Marianetti
Phys. Rev. Lett. 111, 116403 (2013)

17. *Investigation of Non-linear Elastic Behavior of Two-Dimensional Molybdenum Disulfide*
R.C. Cooper, C. Lee, C.A. Marianetti, X. Wei, J. Hone, and J.W. Kysar
Phys. Rev. B 87, 035423 (2013)

18. *Spin-exchange-induced dimerization of an atomic 1-D system*
N. Zaki, C.A. Marianetti, D.P. Acharya, P. Zahl, P. Sutter, J. Okamoto, P.D. Johnson, A.J. Millis, R.M. Osgood
Phys. Rev. B 87, 161406(R) (2013)

19. *Site-selective Mott transition in rare earth nickelates*
H. Park, A.J. Millis, C.A. Marianetti
Phys. Rev. Lett. 109, 156402 (2012)

20. *Measurement of the phonon density of states of PuO_2(+2% Ga): A critical test of theory*
M.E. Manley, J.R. Jeffries, A.H. Said, C.A. Marianetti, H. Cynn, B.M. Leu, and M.A. Wall
Phys. Rev. B 85, 132301 (2012)

21. *Covalency, double-counting and the metal-insulator phase diagram in transition metal oxides*
X. Wang, M.J. Han, L. deMedici, H. Park, C.A. Marianetti, A.J. Millis
Phys. Rev. B 86, 195136 (2012)

22. *Dynamical Mean Field Theory of Nickelate Superlattices*
M.J. Han, X. Wang, C.A. Marianetti, and A.J. Millis

Phys. Rev. Lett. 107, 206804 (2011)

23. *Dynamical Mean-Field Theory for Quantum Chemistry*
N. Lin, C.A. Marianetti, A.J. Millis, and D.R. Reichman
Phys. Rev. Lett. 106, 096402 (2011)

24. *Failure mechanisms of graphene under tension*
C.A. Marianetti and H.G. Yevick
Phys. Rev. Lett. 105, 245502 (2010)

25. *Chemical Control of Orbital Polarization in Artificially Structured Transition Metal Oxide Materials: the case of La2NiXO6*
M.J. Han, C.A. Marianetti and A.J. Millis
Phys. Rev. B 82, 134408 (2010)

26. *Nonlinear elastic behavior of graphene: Ab initio calculations to continuum description*
X. Wei, B. Fragneaud, C.A. Marianetti, and J.W. Kysar
Phys. Rev. B 80, 205407 (2009)

27. *Electronic coherence in delta-Pu: A DMFT study.*
C.A. Marianetti, K. Haule, G. Kotliar, and M.J. Fluss
Phys. Rev. Lett. 101, 056403 (2008)

28. *A dynamical mean-field theory study of Nagaoka ferromagnetism.*
H. Park, K. Haule, C.A. Marianetti, and G. Kotliar
Phys. Rev. B 77, 035107 (2008)

29. *One-electron physics of the actinides*
A. Toropova, C.A. Marianetti, K. Haule, and G. Kotliar
Phys. Rev. B 76, 155126 (2007)

30. *Quasiparticle dispersion and heat capacity of Na0.3CoO2: A DMFT study*
C.A. Marianetti, O. Parcollet, and K. Haule
Phys. Rev. Lett. 99, 246404 (2007)

31. *Na induced correlations in the cobaltates.*
C.A. Marianetti and G. Kotliar
Phys. Rev. Lett. 98, 176405 (2007)

32. *Electronic structure calculations with dynamical mean-field theory.*
G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti
Rev. Mod. Phys. 78, 865 (2006)

33. *A first-order Mott transition in LixCoO2.*
C.A. Marianetti, G. Kotliar, G. Ceder
Nature Materials Vol. 3, Page 627 (2004)

34. *Role of hybridization in NaxCoO2 and the effect of hydration.*
C.A. Marianetti, G. Kotliar, G. Ceder
Phys. Rev. Lett. 92, 196405 (2004)

35. *Phase separation in LixFePO4 induced by correlation effects.*
F. Zhou, C. A. Marianetti, M. Cococcioni, D. Morgan, G. Ceder
Phys. Rev. B 201101R, (2004)

36. *First-principles prediction of redox potentials in transition metal compounds with LDA+U.*
Fei Zhou, Matteo Cococcioni, C. A. Marianetti, Dane Morgan, G. Ceder
Phys. Rev. B 70, 235121 (2004)

37. *S = 1/2 chains and spin-Peierls transition in TiOCl.*
A. Seidel, C. A. Marianetti, F. C. Chou, G. Ceder, and P. A. Lee
Phys. Rev. B 67, 020405(R) (2003)

38. *First-Principles study of the stability and electronic structure of metal hydrides.*
H. Smithson, C. A. Marianetti, D. Morgan, A. Van der Ven, A Predith and G. Ceder
Phys. Rev. B 66,144107 (2002)

39. *First-Principles investigation of the cooperative Jahn-Teller Effect for octahedrally coordinated transition-metal oxides.*
C.A. Marianetti, D. Morgan, G. Ceder
Phys. Rev. B 63, 224304 (2001)

40. *Jahn-Teller mediated ordering in layered LixMO2 compounds.*
M. E. Arroyo y de Dompablo, C. Marianetti, A. Van der Ven, and G. Ceder
Phys. Rev. B 63, 144107 (2001)

41. *Phase transformations and volume changes in spinel LixMn2O4.*
Van der Ven A, Marianetti C, Morgan D, Ceder G
Solid State Ionics 135 (1-4): 21-32 Sp. Iss. SI NOV 2000

42. *First-principles alloy theory in oxides.*
Ceder G, Van der Ven A, Marianetti C, Morgan D
Modelling and Simulation in Mat. Sci. and Eng. 8 (3): 311-321 MAY 2000

Invited Talks

1. *Emergent Phenomena in Oxide Superlattices from DFT+DMFT*
Meeting of the American Physical Society,
March 2015, San Antonio, TX

2. *DFT+DMFT total energy calculations in the rare-earth Nickelates*
CECAM Workshop
June 2014, Lausanne, Switzerland

3. *Computing the properties of the rare-earth nickelates via DFT+DMFT*
National Institute of Standards and Technology
May 2014, Maryland

4. *Soft phonon modes in strained monolayer materials*
University of Maryland, Physics Seminar
May 2014, College Park, Maryland

5. *DFT+DMFT calculations in oxide superlattices*
   Meeting of the American Physical Society,
   March 2014, Denver Co

6. *Novel Functionality in oxides via Jahn-Teller ions: a DFT+DMFT study*
   DARPA Cold Atom program review
   Feb 2014, Washington DC

7. *Computing the Phase Stability of Rare-Earth Nickelates via DFT+DMFT*
   Meeting of the Materials Research Society
   12/5/2013, Boston MA

8. *Computing the properties of strongly correlated electron systems via DFT+DMFT*
   Cornell Univeristy Applied Physics Seminar
   10/28/2013, Ithaca NY

9. *Computing the phase stability of rare-earth nickelates via DFT+DMFT*
   CINT Users Conference
   9/25/2013, Santa Fe, NM

10. *Computing Materials Properties from First-Principles*
    West Point Academy Physics Seminar
    9/13/2013, West Point, NY

11. *Computing the phase diagram of the rare-earth Nickelates*
    Mott MURI Annual Review
    August 7th 2013, Stanford, CA

12. *Computing the properties of Complex Oxides using DFT+DMFT*
    March Meeting Tutorial on Complex Oxides
    March 17th 2013
    Baltimore, MD

13. *Computing the properties of SCES using DFT+DMFT*
    Bariloche Workshop on Materials Design
    February 22nd 2013
    Bariloche, Argentina

14. *Multiferroic and Correlated Materials through Ab Initio Design*
    FAME Grant kickoff meeting
    February 5th 2013
    Los Angeles, CA

15. *Computing the phase diagram of the rare-earth Nickelates*
    Meeting on Theory of Complex Oxide Interfaces
    January 21st, 2013
    Argonne National Laboratory

16. *Ideal strength of monolayer materials*
    Drexel University Materials Science Seminar

December 2012,Philadelphia, PA

17. *Soft phonon modes in monolayers*
UT Austin Physics Seminar
October 2012,Austin, Texas

18. *Site-selective Mott transition in rare-earth Nickelates*
Complex Oxide Heterostructure Workshop
August 2012,Cambridge, MA

19. *Site-selective Mott transition in rare-earth Nickelates*
Oxide Interfaces by Design Workshop
July 2012,Newport, RI

20. *Computing the phonons of PuO_2*
Dual Nature of f-Electrons
July 2012,Himeji, Japan

21. *Site-selective Mott transition in rare-earth Nickelates*
Tokyo University
June 2012,Tokyo, Japan

22. *DFT+DMFT - Complex Oxides*
March Meeting Tutorial on Complex Oxides
March 2012,Boston, MA

23. *Hybridization wave induced site-selective mott transition in the nickelates*
Mott MURI Meeting
February 2012,Santa Barbara, CA

24. *Failure mechanisms of graphene*
A workshop to promote the use of high-energy x-ray diffraction experiments and detailed computational analyses for understanding multiscale phenomena in crystalline materials
October 2011,Argonne National Lab

25. *On the metal-insulator transition in TMOs: A DFT+DMFT study*
Oxide Interfaces Meeting
August 2011,Almaden CA

26. *Failure mechanisms of graphene*
ArmorCon Military Armor Conference
June 2011,Washington DC

27. *On the metal-insulator transition in TMOs: A DFT+DMFT study*
Conference on Complex Oxide Heterostructures
April 2011,Las Vegas, Nevada

28. *Chemical Control of Orbital Polarization in the Nickelates*
Complex Oxide workshop
August 2010,University of Virginia

29. *Failure mechanisms of graphene*
Materials Research Society Fall Meeting
November 2010,Boston, MA

30. *Capturing the double well of Pu*
Pu Futures
September 2010,Keystone, CO

31. *Capturing the double well of Pu*
CECAM meeting - Actinides: Correlated electrons and nuclear materials
June 2010,Manchester, England

32. *Predicting Materials Properties using DFT and DMFT*
238th American Chemical Society National Meeting
August 2009,Washington, DC

33. *Electronic coherence in δ-Pu: A DMFT study*
US/Russian Workshop
September 2008,Snezhinsk, Russia

34. *Electronic coherence in δ-Pu: A DMFT study*
Plutonium Futures 2008 Conference
July 2008,Dijon (France)

35. *Electronic properties of the cobaltates*
Princeton University Physics Seminar
April 2008,Princeton, NJ

36. *DMFT calculations of materials properties using the continuous time QMC method*
American Physical Society March Meeting
March 2008,New Orleans, LA

37. *The Fermi surface and heat capacity in $Na_{0.3}CoO_2$*
UC Davis Physics Seminar
November 2007,Davis, CA

38. *Electronic properties of Pu via the dynamical-mean field theory*
CMSN Meeting
September 2007,Davis, CA

39. *ARPES and heat capacity in $Na_{0.3}CoO_2$*
PASI 2007 - Electronic States and Excitations on Nanostructures
June 2007,Zacatecas, Mexico

40. *A DFT+DMFT approach to the electronic structure of the cobaltates*
Boston College Physics Seminar
December 2006,Boston, MA

41. *Correlations in the cobaltates*
First International Workshop on the Physical Properties of Layered Cobaltates
July 2006,Orsay (France)