

# 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

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**Publications: H-Index=21, Total Citations=2363** [Google Scholar 8/4/2014]

1. *Origin of Spinel Nanocheckerboards via First Principles*  
M. Kornbluth and C.A. Marianetti  
arXiv:1501.03480 (2015)
2. *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)
3. *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)
4. *Selectively Localized Wannier Functions*  
R. Wang, E.A. Lazar, H. Park, A.J. Millis, and C.A. Marianetti  
Phys. Rev. B 90, 165125 (2014)
5. *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)
6. *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)
7. *A slave mode expansion for obtaining ab-initio interatomic potentials*  
X. Ai, Y. Chen, and C.A. Marianetti  
Phys. Rev. B 90, 014308 (2014)
8. *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)
9. *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)
10. *Ideal strength and phonon instability of strained monolayer materials*  
E.B. Isaacs and C.A. Marianetti  
Phys. Rev. B 89, 184111 (2014)
11. *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)

12. *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)
13. *Physical adsorption and Charge Transfer of molecular Br<sub>2</sub> 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)
14. *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)
15. *Engineering Correlation Effects via Artificially Designed Oxide Superlattices*  
H. Chen, A.J. Millis, and C.A. Marianetti  
Phys. Rev. Lett. 111, 116403 (2013)
16. *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)
17. *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)
18. *Site-selective Mott transition in rare earth nickelates*  
H. Park, A.J. Millis, C.A. Marianetti  
Phys. Rev. Lett. 109, 156402 (2012)
19. *Measurement of the phonon density of states of PuO<sub>2</sub>(+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)
20. *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)
21. *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)
22. *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)

23. *Failure mechanisms of graphene under tension*  
C.A. Marianetti and H.G. Yevick  
Phys. Rev. Lett. 105, 245502 (2010)
24. *Chemical Control of Orbital Polarization in Artificially Structured Transition Metal Oxide Materials: the case of  $La_2NiXO_6$*   
M.J. Han, C.A. Marianetti and A.J. Millis  
Phys. Rev. B 82, 134408 (2010)
25. *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)
26. *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)
27. *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)
28. *One-electron physics of the actinides*  
A. Toropova, C.A. Marianetti, K. Haule, and G. Kotliar  
Phys. Rev. B 76, 155126 (2007)
29. *Quasiparticle dispersion and heat capacity of  $Na_{0.3}CoO_2$ : A DMFT study*  
C.A. Marianetti, O. Parcollet, and K. Haule  
Phys. Rev. Lett. 99, 246404 (2007)
30. *Na induced correlations in the cobaltates.*  
C.A. Marianetti and G. Kotliar  
Phys. Rev. Lett. 98, 176405 (2007)
31. *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)
32. *A first-order Mott transition in  $Li_xCoO_2$ .*  
C.A. Marianetti, G. Kotliar, G. Ceder  
Nature Materials Vol. 3, Page 627 (2004)
33. *Role of hybridization in  $NaxCoO_2$  and the effect of hydration.*  
C.A. Marianetti, G. Kotliar, G. Ceder  
Phys. Rev. Lett. 92, 196405 (2004)
34. *Phase separation in  $Li_xFePO_4$  induced by correlation effects.*  
F. Zhou, C. A. Marianetti, M. Cococcioni, D. Morgan, G. Ceder  
Phys. Rev. B 201101R, (2004)
35. *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)
36. *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)
  37. *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)
  38. *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)
  39. *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)
  40. *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
  41. *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. *DFT+DMFT total energy calculations in the rare-earth Nickelates*  
CECAM Workshop  
June 2014, Lausanne, Switzerland
2. *Computing the properties of the rare-earth nickelates via DFT+DMFT*  
National Institute of Standards and Technology  
May 2014, Maryland
3. *Soft phonon modes in strained monolayer materials*  
University of Maryland, Physics Seminar  
May 2014, College Park, Maryland
4. *DFT+DMFT calculations in oxide superlattices*  
Meeting of the American Physical Society,  
March 2014, Denver Co
5. *Novel Functionality in oxides via Jahn-Teller ions: a DFT+DMFT study*  
DARPA Cold Atom program review  
Feb 2014, Washington DC
6. *Computing the Phase Stability of Rare-Earth Nickelates via DFT+DMFT*  
Meeting of the Materials Research Society

- 12/5/2013, Boston MA
7. *Computing the properties of strongly correlated electron systems via DFT+DMFT*  
Cornell University Applied Physics Seminar  
10/28/2013, Ithaca NY
  8. *Computing the phase stability of rare-earth nickelates via DFT+DMFT*  
CINT Users Conference  
9/25/2013, Santa Fe, NM
  9. *Computing Materials Properties from First-Principles*  
West Point Academy Physics Seminar  
9/13/2013, West Point, NY
  10. *Computing the phase diagram of the rare-earth Nickelates*  
Mott MURI Annual Review  
August 7th 2013, Stanford, CA
  11. *Computing the properties of Complex Oxides using DFT+DMFT*  
March Meeting Tutorial on Complex Oxides  
March 17th 2013  
Baltimore, MD
  12. *Computing the properties of SCES using DFT+DMFT*  
Bariloche Workshop on Materials Design  
February 22nd 2013  
Bariloche, Argentina
  13. *Multiferroic and Correlated Materials through Ab Initio Design*  
FAME Grant kickoff meeting  
February 5th 2013  
Los Angeles, CA
  14. *Computing the phase diagram of the rare-earth Nickelates*  
Meeting on Theory of Complex Oxide Interfaces  
January 21st, 2013  
Argonne National Laboratory
  15. *Ideal strength of monolayer materials*  
Drexel University Materials Science Seminar  
December 2012, Philadelphia, PA
  16. *Soft phonon modes in monolayers*  
UT Austin Physics Seminar  
October 2012, Austin, Texas
  17. *Site-selective Mott transition in rare-earth Nickelates*  
Complex Oxide Heterostructure Workshop  
August 2012, Cambridge, MA

18. *Site-selective Mott transition in rare-earth Nickelates*  
Oxide Interfaces by Design Workshop  
July 2012, Newport, RI
19. *Computing the phonons of PuO<sub>2</sub>*  
Dual Nature of f-Electrons  
July 2012, Himeji, Japan
20. *Site-selective Mott transition in rare-earth Nickelates*  
Tokyo University  
June 2012, Tokyo, Japan
21. *DFT+DMFT - Complex Oxides*  
March Meeting Tutorial on Complex Oxides  
March 2012, Boston, MA
22. *Hybridization wave induced site-selective mott transition in the nickelates*  
Mott MURI Meeting  
February 2012, Santa Barbara, CA
23. *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
24. *On the metal-insulator transition in TMOs: A DFT+DMFT study*  
Oxide Interfaces Meeting  
August 2011, Almaden CA
25. *Failure mechanisms of graphene*  
ArmorCon Military Armor Conference  
June 2011, Washington DC
26. *On the metal-insulator transition in TMOs: A DFT+DMFT study*  
Conference on Complex Oxide Heterostructures  
April 2011, Las Vegas, Nevada
27. *Chemical Control of Orbital Polarization in the Nickelates*  
Complex Oxide workshop  
August 2010, University of Virginia
28. *Failure mechanisms of graphene*  
Materials Research Society Fall Meeting  
November 2010, Boston, MA
29. *Capturing the double well of Pu*  
Pu Futures  
September 2010, Keystone, CO

30. *Capturing the double well of Pu*  
CECAM meeting - Actinides: Correlated electrons and nuclear materials  
June 2010, Manchester, England
31. *Predicting Materials Properties using DFT and DMFT*  
238th American Chemical Society National Meeting  
August 2009, Washington, DC
32. *Electronic coherence in  $\delta$ -Pu: A DMFT study*  
US/Russian Workshop  
September 2008, Snezhinsk, Russia
33. *Electronic coherence in  $\delta$ -Pu: A DMFT study*  
Plutonium Futures 2008 Conference  
July 2008, Dijon (France)
34. *Electronic properties of the cobaltates*  
Princeton University Physics Seminar  
April 2008, Princeton, NJ
35. *DMFT calculations of materials properties using the continuous time QMC method*  
American Physical Society March Meeting  
March 2008, New Orleans, LA
36. *The Fermi surface and heat capacity in  $\text{Na}_{0.3}\text{CoO}_2$*   
UC Davis Physics Seminar  
November 2007, Davis, CA
37. *Electronic properties of Pu via the dynamical-mean field theory*  
CMSN Meeting  
September 2007, Davis, CA
38. *ARPES and heat capacity in  $\text{Na}_{0.3}\text{CoO}_2$*   
PASI 2007 - Electronic States and Excitations on Nanostructures  
June 2007, Zacatecas, Mexico
39. *A DFT+DMFT approach to the electronic structure of the cobaltates*  
Boston College Physics Seminar  
December 2006, Boston, MA
40. *Correlations in the cobaltates*  
First International Workshop on the Physical Properties of Layered Cobaltates  
July 2006, Orsay (France)