Chris A. Marianetti

Associate Professor of Materials Science
and Applied Physics and Applied Mathematics
Columbia University
chris.marianetti@columbia.edu
http://www.chrismarianetti.org

500 West 120th Street
1144 Mudd Hall
New York, NY 10027
(212) 854-9478

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

Zhengqian Cheng, Lyuwen Fu, Enda Xiao, Mark Mathis

Current Postdocs

None.

Professional Societies

American Physical Society, Materials Research Society, American Chemical Society.

Editor

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

Publications: H-Index=30, Total Citations=5356 [Google Scholar 4/12/2019]

1. *Compositional phase stability of correlated electron materials within DFT+DMFT*
   E.B. Isaacs and C.A. Marianetti
   ArXiv 1903.10436 (2019)

2. *Structural and metal-insulator transitions in rhenium based double perovskites via orbital ordering*
   T. Lee and C.A. Marianetti
   Phys. Rev. B 97, 045102 (2018)

3. *Signatures of the topological s+- superconducting order parameter in the type-II Weyl semimetal Td-MoTe2*
   Z. Guguchia, F. von Rohr, Z. Shermadini, A. T. Lee, S. Banerjee, A. R. Wieteska, C. A. Marianetti, B. A. Frandsen, H. Luetkens, Z. Gong, S. C. Cheung, C. Baines, A. Shengelaya, G. Taniashvili, A. N. Pasupathy, E. Morenzoni, S. J. L. Billinge, A. Amato, R. J. Cava, R. Khasanov, and Y. J. Uemura
   Nature Communications 8, 1082 (2017)

4. *Compositional phase stability of strongly correlated electron materials within DFT+U*
   E.B. Isaacs and C.A. Marianetti
   Phys. Rev. B 95, 045141 (2017)

5. *Electronic correlations in monolayer VS2*
   E.B. Isaacs and C.A. Marianetti
   Phys. Rev. B 94, 035120 (2016)

6. *Influence of quantum confinement and strain on orbital polarization of four-layer LaNiO3 superlattices: a DFT+DMFT study*
   H. Park, A.J. Millis, and C.A. Marianetti
   Phys. Rev. B 93, 235109 (2016)

7. *Applicability of DFT + U to U metal and U-Zr alloy*
   W. Xie, C.A. Marianetti, and D. Morgan
   arXiv 1601.07959v1

8. *Pressure-resistant intermediate valence in Kondo insulator SmB6*
   N.P. Butch, J. Paglione, P. Chow, Y. Xiao, C.A. Marianetti, C.H. Booth, J.R. Jeffries
   Phys. Rev. Lett. 116, 156401 (2016)

9. *New class of planar ferroelectric Mott insulators via first principles design*
   C. Kim, H. Park, and C.A. Marianetti
   Phys. Rev. B 92, 235122 (2015)

10. *Density functional versus spin-density functional and the choice of correlated subspace in multi-variable effective action theories of electronic structure*
    H. Park, A.J. Millis, and C.A. Marianetti
    Phys. Rev. B 92, 035146 (2015)

11. *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
    Phys. Rev. B 91, 241111 (2015)

12. *Origin of Spinel Nanocheckerboards via First Principles*
    M. Kornbluth and C.A. Marianetti
    Phys. Rev. Lett. 114, 226102 (2015)

13. *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)

14. *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)

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

16. *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)

17. *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)

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

19. *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)

20. *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)

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

22. *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)

23. *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)

24. *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)

25. *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)

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

27. *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)

28. *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)

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

30. *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)

31. *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)

32. *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)

33. *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)

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

35. *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)

36. *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)

37. *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)

38. *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)

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

40. *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)

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

42. *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)

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

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

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

46. *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)

47. *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)

48. *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)

49. *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)

50. *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)

51. *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

52. *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. *Multi-projective variational approach to the quantum lattice problem*
Meeting of the American Chemical Society
April 2019 Orlando, Fl

2. *An optimal approach to computing phonons and their interactions via finite difference*
CECAM Workshop - Anharmonicity and thermal properties of solids
January 2018 Paris, France

3. *Structural and metal-insulator transitions in rhenium based double perovskites via orbital ordering*
Queens University
September 2017 Belfast, Ireland

4. *Orbital Ordering in Re-based Double Perovskites*
City College
May 2017 New York, NY

5. *Orbital Ordering in Re-based Double Perovskites*
Conference on Study of Matter at Extreme Conditions
April 2017 Caribbean

6. *Soft phonon modes in strained monolayer materials*
National Cheng Kung University
August 2016, Tainan, Taiwan

7. *Phase diagram of the rare-earth Nickelates from first-principles*
National Cheng Kung University
August 2016, Tainan, Taiwan

8. *Computing the properties of strongly correlated electron materials via DFT+DMFT*
Rutgers Newark, Department of Chemistry
April 2016, Newark, NJ

9. *Interatomic potential for graphene derived from first-principles*
AmeriMech Symposium
April 2016, Austin, Texas

10. *Hubbard operator density functional theory for Fermionic lattice models*
American Chemical Society Meeting
March 2016, San Diego, California

11. *Strong electronic correlations in 2D materials*
Collaborative Conference on Crystal Growth
December 2015, Hong Kong

12. *Computing the properties of strongly correlated electron materials via DFT+DMFT*
Department of Physics seminar at Virginia Tech
November 2015, Virginia Tech

13. *Lighting the way for complex materials*
Advanced Photon Source Upgrade Conference
May 2015, Argonne National Laboratory

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

29. *Ideal strength of monolayer materials*
Drexel University Materials Science Seminar
December 2012,Philadelphia, PA

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

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

32. *Site-selective Mott transition in rare-earth Nickelates*
Oxide Interfaces by Design Workshop

July 2012,Newport, RI

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

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

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

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

37. *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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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