Chris Marianetti
Professor
Dept. of Applied Physics and Applied Mathematics
Columbia University

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Research Interests

Professor Marianetti's research field is an intersection of materials science and quantum many-body physics, with focus on various techniques and materials, including density functional theory, dynamical mean-field theory, the variational discrete action theory, energy generation/storage materials, strongly correlated electrons, phonon interactions, actinides, transition-metal oxides, and monolayer materials.

Education

Massachusetts Institute of Technology
Ph.D., Materials Science and Engineering, 2004

The Ohio State University
M.S., Welding Engineering, 1998

The Ohio State University
B.S., Welding Engineering, 1997

Employment

Columbia University
Professor of Materials Science and Applied Physics and Applied Mathematics
Department of Applied Physics and Applied Mathematics
January 2025-Present

Columbia University
Associate Professor of Materials Science and Applied Physics and Applied Mathematics
Department of Applied Physics and Applied Mathematics
July 2013-December 2024

Columbia University
Assistant Professor of Materials Science and Applied Physics and Applied Mathematics
Department of Applied Physics and Applied Mathematics
July 2008-June 2013

Lawrence Livermore National Laboratory
Postdoctoral Researcher
Materials and Chemistry
July 2007-July 2008

Rutgers University
Postdoctoral Researcher
Department of Physics, Feb 2004-June 2007

Major Awards

NSF Career Award (2012)
DARPA Young Faculty Award (2013)

Professional Societies

American Physical Society

Teaching and Education Experience

Former Postdoctoral Researchers

- Myung Joon Han - Associate Professor of Physics at KAIST.
- Hyowon Park - Assistant Professor of Physics at University of Illinois at Chicago with a joint appointment at Argonne National Lab.
- Yue Chen - Associate Professor of Materials at Hong Kong University.
- Pierre Darancet - Assistant Scientist, Argonne National Laboratory.
- Emanuel Lazar - Senior Lecturer, Bar-Ilan University.
- Jia Chen - Head of Quantum Research at QSimulate.
- Dalal Kanan - Visiting Assistant Professor at Fordham University.
- Alex Taekyung Lee - Postdoctoral Researcher at Yale.

Current Postdoctoral Researchers

- Zhengqian Cheng

Graduated PhD Students

- Xinyuan Ai (2015) - Assistant Professor at Hunan University.
  Slave mode expansion for obtaining ab initio interatomic potentials and its applications
- Eric Isaacs (2016) - Staff scientist at Hughes Research Lab.
  Electronic structure and phase stability of strongly correlated electron materials
- Mordechai Kornbluth (2017) - Research Scientist at Bosch.
  Anharmonic phonons in graphene from first principles
- Chanul Kim (2018) - Consultant at Bain & Company.
  Predicting the temperature-strain phase diagram of VO_2 from first principles
- Zhengqian Cheng (2021) - Postdoctoral researcher at Columbia University.
  Variational discrete action theory
- Lyuwen Fu (2021) - Research Scientist at Zhejiang Lab.
  Thermodynamics of interacting phonons
- Enda Xiao (2023) - Postdoctoral researcher at National Institute for Materials Science.
  Anharmonic Phonon Behavior using Hamiltonians constructed via Irreducible Derivatives

- Mark Mathis (2024) - Postdoctoral researcher at Los Alamos National Laboratory.
  Crystal vibrations at finite strain and stress within the generalized quasiharmonic approximation
- Sasaank Bandi (2024) - Postdoctoral researcher at Sandbox AQ.
  The Construction of Robust Potential Energy Surfaces from First Principles and Machine Learning

Current PhD Students

Shenwei Wu (2027), Ruining Zhang (2027), and Seungbin Han (2029).

PhD Thesis Committee Member

Jonathon Karp, Zeyu Hui, Yeongsu Cho, Jonathan Fetherolf, Malte Lange, Matthew Carbone, Long Yang, E-Dean Fung, Shaowen Chen, Peijie Ong, Chia-Hao Liu, Chris DiMarco, Chris Wright, Drew Edelberg, Qiang Han, Vernon Wong, Runzhi Wang, Andrew Weisman, Antonio Levy, Wencan Jin, Sophie Chauvin, Ying Wang, Jin Wang, Xiaohao Yang, Ethan Rosenthal, Seyoung Park, Arun Batra, Sriharsha Aradhya, Dory Kramer, Jing Zhang, Austin Akey, Anil Raj, Timur Dykhne, Charlton Chen, Yuri Zuev, Sioan Zohar, Jun Yan, Joanna Atkin.

Publications

H-Index=40, Total Citations=10,282 [Google Scholar 2/2/2025]

(Students and postdocs funded by Marianetti are underlined; senior author last.)

1. *Ab initio elasticity at finite temperature and stress in ferroelectrics*
   M.A. Mathis and **C.A. Marianetti**
   Phys. Rev. B 110, L140101 (2024)
2. *Benchmarking phonon anharmonicity in machine learning interatomic potentials*
   S. Bandi, C. Jiang, and **C.A. Marianetti**
   Mach. Learn.: Sci. Technol. 5, 030502 (2024)
3. *Phonon thermal transport in UO_2 via self-consistent perturbation theory*
   S. Zhou, E. Xiao, H. Ma, K. Gofryk, C. Jiang, M. E. Manley, D. H. Hurley, and **C. A. Marianetti**
   Phys. Rev. Lett. 132, 106502 (2024)
4. *First-principles determination of the phonon-point defect scattering and thermal transport due to fission products in ThO_2*
   L. Malakkal, Ankita Katre, S. Zhou, C. Jiang, D. H. Hurley, **C. A. Marianetti**, M. Khafizov
   Phys. Rev. Mater. 8, 025401 (2024)
5. *Machine learning potential assisted exploration of complex defect potential energy surfaces*
   C. Jiang, **C. A. Marianetti**, M. Khafizov, and D. H. Hurley
   NPG Computational Materials 10, 21 (2024)

6. *Magnetism and Metallicity in Moire Transition Metal Dichalcogenides*
P. Tscheppe, J. Zang, M. Klett, S. Karakuzu, A. Celarier, Z. Cheng, **C. A. Marianetti**, T. A. Maier, M. Ferrero, A. J. Millis, T. Schafer
Proceedings of the National Academy of Sciences 121, e2311486121 (2024)

7. *Impacts of irradiation-induced nanostructure on phonon linewidths and thermal conductivity in U-Zr alloy*
H. Ma, Z. Hua, A. Sen, T. Yao, M. S. Bryan, A. Alatas, E. K. Nosal, S. Adnan, E. Xiao, A. French, M. Bachhav, **C. A. Marianetti**, M. Khafizov, L. Shao, L. He, J. P. Wharry, D. H. Hurley, and M. E. Manley
Phys. Rev. B 108, 104318 (2023)

8. *A gauge constrained algorithm of VDAT at $\mathcal{N} = 3$ for the multi-orbital Hubbard model*
Z. Cheng and **C. A. Marianetti**
Phys. Rev. B 108, 035127 (2023)

9. *Precisely computing phonons via irreducible derivatives*
S. Bandi and **C. A. Marianetti**
Phys. Rev. B 107, 174302 (2023)

10. *Anharmonic phonon behavior via irreducible derivatives: self-consistent perturbation theory and molecular dynamics*
E. Xiao and **C. A. Marianetti**
Phys. Rev. B 107, 094303 (2023)

11. *Precise ground state of multi-orbital Mott systems via the variational discrete action theory*
Z. Cheng and **C. A. Marianetti**
Phys. Rev. B 106, 205129 (2022)

12. *Advances in actinide thin films: synthesis, properties, and future directions*
K. D. Vallejo, F. Kabir, N. Poudel, **C. A. Marianetti**, D. H. Hurley, P. J. Simmonds, C. A. Dennett, K. Gofryk
Rep. Prog. Phys. 85 123101 (2022)

13. *Capturing the ground state of uranium dioxide from first principles: crystal distortion, magnetic structure, and phonons*
S. Zhou, H. Ma, E. Xiao, K. Gofryk, C. Jiang, M. E. Manley, D. H. Hurley, **C. A. Marianetti**
Phys. Rev. B 106, 125134 (2022)

14. *Validating First-Principles Phonon Lifetimes via Inelastic Neutron Scattering*
E. Xiao, H. Ma, M.S. Bryan, L. Fu, J.M. Mann, B. Winn, D.L. Abernathy, R.P. Hermann, A.R. Khanolkar, C.A. Dennett, D.H Hurley, M.E. Manley, and **C. A. Marianetti**
Phys. Rev. B 106, 144310 (2022)

15. *The generalized quasiharmonic approximation via space group irreducible derivatives*
M. A. Mathis, A. Khanolkar, L. Fu, M. S. Bryan, C. A. Dennett, K. Rickert, J. M.

Mann, B. Winn, D. L. Abernathy, M. E. Manley, D. H. Hurley, **C. A. Marianetti**
Phys. Rev. B 106, 014314 (2022)

16. *Thermal Energy Transport in Oxide Nuclear Fuel*
D.H. Hurley, A. El-azab, M.S. Bryan, M. Cooper, C.A. Dennett, K. Gofryk, L.F. He, M. Khafizov, G.H. Lander, M.E. Manley, J.M. Mann, **C. A. Marianetti**, K. Rickert, F.A. Selim, M.R. Tonks, and J.P. Wharry
Chem. Rev. 122, 3711 (2022)

17. *Assessment of empirical interatomic potential to predict thermal conductivity in ThO_2 and UO_2*
M.M. Jin, M. Khafizov, C. Jiang, S.X. Zhou, **C. A. Marianetti**, M.S. Bryan, M.E. Manley, and D.H. Hurley
Journal of Physics - Condensed Matter 33, 275402 (2021)

18. *An integrated experimental and computational investigation of defect and microstructural effects on thermal transport in thorium dioxide*
C.A. Dennett, W.R. Deskins, M. Khafizov, Z. Hua, A. Khanolkar, K. Bawane, L. Fu, J.M. Mann, **C. A. Marianetti**, L. He, D.H. Hurley, and A. El-Azab
Acta Materialia 213, 116934 (2021)

19. *Variational Discrete Action Theory*
Z. Cheng and **C. A. Marianetti**
Phys. Rev. Lett. 126, 206402 (2021)

20. *Foundations of Variational Discrete Action Theory*
Z. Cheng and **C. A. Marianetti**
Phys. Rev. B 103, 195138 (2021)

21. *Magnetic, transport and thermal properties of delta-phase UZr_2*
X. Ding, T. Yao, L. Fu, Z. Hua, J. Harp, **C. A. Marianetti**, M. Neupane, M.E. Manley, D. Hurley, and K. Gofryk
Philosophical Magazine Letters 101, 1 (2021)

22. *Nonlinear propagating modes beyond the phonons in fluorite-structured crystals*
M.S. Bryan, L. Fu, K. Rickert, D. Turner, T.A. Prusnick, J.M. Mann, D.L. Abernathy, **C. A. Marianetti** , and M.E. Manley
Communications Physics 3, 217 (2020)

23. *Compositional phase stability of correlated electron materials within DFT+DMFT*
E.B. Isaacs and **C. A. Marianetti**
Phys. Rev. B 102, 045146 (2020)

24. *Off-shell effective energy theory: a unified treatment of the Hubbard model from d=1 to d=∞*
Z. Cheng and **C. A. Marianetti**
Phys. Rev. B 101, 081105(R) (2020)

25. *A group theoretical approach to computing phonons and their interactions*
L. Fu, M. Kornbluth, Z. Cheng, and **C. A. Marianetti**

Phys. Rev. B 100, 014303 (2019)

26. *Approaching the Intrinsic Limit in Transition Metal Diselenides via Point Defect Control*
D. Edelberg, D. Rhodes, A. Kerelsky, B. Kim, J. Wang, A. Zangiabadi, C. Kim, A. Abhinandan, J. Ardelean, M. Scully, D. Scullion, L. Embon, R. Zu, E. Santos, L. Balicas, **C. A. Marianetti**, K. Barmak, X.Y. Zhu, J. Hone, and A.N. Pasupathy
Nano Letters 19, 4371 (2019)

27. *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)

28. *Signatures of the topological s^{+-} superconducting order parameter in the type-II Weyl semimetal Td-$MoTe_2$*
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)

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

30. *Electronic correlations in monolayer VS_2*
E.B. Isaacs and **C. A. Marianetti**
Phys. Rev. B 94, 035120 (2016)

31. *Influence of quantum confinement and strain on orbital polarization of four-layer $LaNiO_3$ superlattices: a DFT+DMFT study*
H. Park, A.J. Millis, and **C. A. Marianetti**
Phys. Rev. B 93, 235109 (2016)

32. *Pressure-resistant intermediate valence in Kondo insulator SmB_6*
N.P. Butch, J. Paglione, P. Chow, Y. Xiao, **C. A. Marianetti**, C.H. Booth, J.R. Jeffries
Phys. Rev. Lett. 116, 156401 (2016)

33. *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)

34. *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)

35. *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)

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

37. *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)

38. *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)

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

40. *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)

41. *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)

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

43. *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)

44. *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)

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

46. *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)

47. *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)

48. *Physical adsorption and Charge Transfer of molecular Br_2 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)

49. *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)

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

51. *Nonlinear 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)

52. *Experimental observation of 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)

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

54. *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)

55. *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)

56. *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)

57. *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)

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

59. *Chemical Control of Orbital Polarization in Artificially Structured Transition Metal Oxide Materials: the case of* $La_2Ni_XO_6$
M.J. Han, **C. A. Marianetti** and A.J. Millis
Phys. Rev. B 82, 134408 (2010)

60. *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)

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

62. *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)

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

64. *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)

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

66. *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)

67. *A first-order Mott transition in* Li_xCoO_2*.*
C. A. Marianetti, G. Kotliar, G. Ceder
Nature Materials Vol. 3, Page 627 (2004)

68. *Role of hybridization in* Na_xCoO_2 *and the effect of hydration.*
C. A. Marianetti, G. Kotliar, G. Ceder
Phys. Rev. Lett. 92, 196405 (2004)

69. *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)

70. *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)

71. *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)

72. *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)

73. *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)

74. *Jahn-Teller mediated ordering in layered Li_xMO_2 compounds.*
M. E. Arroyo y de Dompablo, **C. Marianetti**, A. Van der Ven, and G. Ceder
Phys. Rev. B 63, 144107 (2001)

75. *Phase transformations and volume changes in spinel $Li_xMn_2O_4$.*
A. Van der Ven, **C. Marianetti** , D. Morgan , G. Ceder
Solid State Ionics 135 (1-4): 21-32 Sp. Iss. SI NOV 2000

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