Marco Bernardi

Professor of Applied Physics, Physics and Materials Science at Caltech

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Research Areas

Computational physics, first-principles calculations

Materials physics, interactions and dynamics in matter

Quantum materials, quantum science and technology

Education

2013 **Ph.D., Materials Science**, *Massachusetts Institute of Technology*, Cambridge, MA

2008 **M.S. Materials Science**, *University of Rome Tor Vergata*, Rome, Italy

2004 **B.S. Chemistry**, *University of Rome La Sapienza*, Rome, Italy

Professional Experience

2021– **Professor**, *Caltech*, Pasadena, CA
Department of Applied Physics and Materials Science, and Department of Physics

2015–2021 **Assistant Professor**, *Caltech*, Pasadena, CA
Department of Applied Physics and Materials Science

2013–2015 **Postdoctoral Scholar**, *UC Berkeley & Berkeley National Laboratory*, Berkeley CA
Department of Physics at UC Berkeley. Advisors: Steven Louie and Jeffrey Neaton

2008–2013 **Research Assistant**, *Massachusetts Institute of Technology (MIT)*, Cambridge MA
Department of Materials Science and Engineering. Advisor: Jeffrey Grossman

Honors and Awards

2026 Fellow of the American Physical Society (APS)

2020 ISSNAF "Franco Strazzabosco" Young Investigator Award

2019 Emerging Young Investigator at 4th Functional Oxide Thin Films Conference

2018 NSF CAREER Award

2017 AFOSR Young Investigator Program (YIP) Award

2015 Psi-K Volker Heine Young Investigator Award

2011 Intel Ph.D. Fellowship

2009 MIT DMSE 1st Year Graduate Student Exceptional Performance Award

2007 Australian Endeavor Research Fellowship

Selected Professional Activities

2026 Committee Member, APS Mildred Dresselhaus Prize

2025 Organizer, Symposium on "Exciton-Phonon Interactions and Ultrafast Dynamics: Theory and Simulations" (DCOMP), APS March Meeting

2025 Chair, Faculty Search Committee, Applied Physics and Materials Science, Caltech

2025 Review Panel, NSF Materials Research Science and Engineering Centers (MRSEC)

2025 Organizer, Perturbo code workshop (every two years since 2020)

2024 Option Representative, Materials Science Program, Caltech (2024–2026)

2024 Organizer, Symposium on "Ultrafast Dynamics From Electron-Phonon Interactions" (DCOMP), APS March Meeting

2023 Visiting Scientist, Scuola Normale Superiore, Pisa, Italy

2023 Reviewer, ASCR Leadership Computing Challenge (ALCC) Proposals

2022 Faculty Search Committee, Applied Physics & Materials Science (2022–2024)

2019 Section Editor, Handbook of Materials Modeling, Springer

2017 Reviewer, PRACE (Partnership for Advanced Computing in Europe) HPC proposals.

2015–2026 Reviewer: Nature, Science, Nature Physics, Nature Materials, Nature Nanotechnology, Nature Communications, Science Advances, Physical Review Letters, Physical Review X, Physical Review B, Physical Review Materials, Nano Letters, ACS Nano, Npj Computational Materials, Npj Quantum Materials, JACS (among others).

2015–2026 Grant Reviewer: US National Science Foundation, US Department of Energy (BES), US Department of Defense, Swiss NSF, DFG German Research Foundation.

Teaching

2016–2026 Electronic and Crystal Structure of Materials (MS 131)

2020–2026 Introduction to Computational Methods for Science and Engineering (APh 141)

2018 Computational Solid State Physics and Materials Science (APh 256)

Mentoring

Graduate Student Advisees

Current: Yao Luo, Sergei Kliavinek, Lauren Tan, Shiv Seshan, Serena Bragadini, Thomas Theiner.

Awards: Yao Luo, 2026 Clauser Prize (best PhD thesis in any field at Caltech); Hsiao-Yi Chen, 2021 Demetriades Prize (best PhD thesis in Nanotechnology)

Former: David Abramovitch (CCQ Flatiron), Khoa Le, Ina Sorensen, Jia Yao, Dhruv Desai (Goldman Sachs), Benjamin Chang (Meta), Jinsoo Park (Postech, Korea), Hsiao-Yi Chen (Tohuku, Japan), Nien-En Lee (MediaTek), I-Te Lu (NYCU, Taiwan), Vatsal Jhalani (NASA JPL).

Postdoctoral Advisees

Current: Tommaso Chiarotti, Ramesh Dhakal

Former: Shiyu Peng (CUHK, Hong Kong), Ivan Maliyov (Microsoft Quantum, Denmark), Sergio Pineda-Flores, Shiyuan Gao, Jin-Jian Zhou (Beijing Tech, China), Luis Agapito (Synopsys), Raffaello Bianco (University of Modena, Italy).

Publications

85 peer-reviewed papers; h-index: 45; >10,000 citations. See Google Scholar

See group website for full publication list.

Selected Publications

1. Y. Luo, J. Park, **M. Bernardi**
   First-principles Diagrammatic Monte Carlo for electron-phonon interactions and polaron.
   Nature Physics **2025** *21*, 1275. DOI: 10.1038/s41567-025-02954-1
   Featured in Caltech News and Physics World.
2. Y. Luo, D. Mantgani, S. Peng, J. Yao, S. Kliavinek, **M. Bernardi**
   Tensor learning and compression of N-Phonon interactions.
   Physical Review Letters **2025** *135*, 126101. DOI: 10.1103/nmgj-yq1g
   Featured in Caltech News
3. Y. Luo, D. Desai, B.K. Chang, J. Park, **M. Bernardi**
   Data-driven compression of electron-phonon interactions.
   Physical Review X **2024** *14*, 021023. DOI: 10.1103/PhysRevX.14.021023
   Featured in Caltech News
4. D.J. Abramovitch, J. Mravlje, J.-J. Zhou, A. Georges, **M. Bernardi**
   Respective roles of electron-phonon and electron-electron interactions
   in the transport and quasiparticle properties of $SrVO_3$.
   Physical Review Letters **2024** *133*, 186501. DOI: 10.1103/PhysRevLett.133.186501
5. D. Abramovitch, J.-J. Zhou, J. Mravlje, A. Georges, **M. Bernardi**
   Combining electron-phonon and dynamical mean field theory calculations of correlated materials: transport in the correlated metal Sr2RuO4. DOI: 10.1103/PhysRevMaterials.7.093801
   Physical Review Materials **2023** *7*, 093801 (Editor's Suggestion).
6. J. Park, J.-J. Zhou, Y. Luo, **M. Bernardi**
   Predicting phonon-induced spin decoherence from first principles:
   colossal spin renormalization in condensed matter.
   Physical Review Letters **2022** *129*, 197201. DOI: 10.1103/PhysRevLett.129.197201
   Featured in Caltech News
7. J.-J. Zhou, J. Park, I. Timrov, A. Floris, M. Cococcioni, N. Marzari and **M. Bernardi**
   Ab Initio electron-phonon interactions in correlated electron systems.
   Physical Review Letters **2021**, *127*, 126404. DOI: 10.1103/PhysRevLett.127.126404
   Highlighted by EPFL Marvel Center.
8. J.-J. Zhou, J. Park, I.-T. Lu, I. Maliyov, X. Tong, and **M. Bernardi**
   PERTURBO: A software package for ab initio electron-phonon interactions, charge transport and ultrafast dynamics.
   Computer Physics Communications **2021** *264*, 107970. DOI: 10.1016/j.cpc.2021.107970
   Featured in Caltech News. See the Perturbo code webpage
9. V. Jhalani, J.-J. Zhou, J. Park, C.E. Dreyer, and **M. Bernardi**
   Piezoelectric electron-phonon interaction from ab initio dynamical quadrupoles:
   impact on charge transport in wurtzite GaN.
   Physical Review Letters **2020**, *125*, 136602. DOI: 10.1103/PhysRevLett.125.136602

10. H.-Y. Chen, D. Sangalli, and **M. Bernardi**
Exciton-phonon interaction and relaxation times from first principles.
Physical Review Letters **2020**, *125*, 107401. DOI: 10.1103/PhysRevLett.125.107401
11. J. Park, J.-J. Zhou, and **M. Bernardi**
Spin-phonon relaxation times in centrosymmetric materials from first principles.
Physical Review B **2020**, *101*, 045202. DOI: 10.1103/PhysRevB.101.045202
12. I.-T. Lu, J.-J. Zhou, and **M. Bernardi**
Efficient ab initio calculations of electron-defect scattering and defect-limited carrier mobility.
Phys. Rev. Mater. **2019**, *3*, 033804 (Editor's Suggestion). DOI: 10.1103/PhysRevMaterials.3.033804
13. J.-J. Zhou, and **M. Bernardi**
Predicting charge transport in the presence of polarons: The beyond-quasiparticle regime in $SrTiO_3$.
Physical Review Research **2019**, *1*, 033138. DOI: 10.1103/PhysRevResearch.1.033138
Featured in Caltech News
14. J.-J. Zhou, O. Hellman and **M. Bernardi**
Electron-phonon scattering in the presence of soft modes
and electron mobility in $SrTiO_3$ perovskite from first principles.
Physical Review Letters **2018**, *121*, 226603. DOI: 10.1103/PhysRevLett.121.226603
15. K. Frohna, T. Deshpande, J. Harter, J. Neaton, S. G. Louie, O. Bakr, D. Hsieh and **M. Bernardi**
Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals.
Nature Communications **2018**, *9*, 1829. DOI: 10.1038/s41467-018-04212-w
Featured in Caltech News
16. V. Jhalani, J.-J. Zhou and **M. Bernardi**
Ultrafast hot carrier dynamics in GaN and its impact on the efficiency droop.
Nano Letters **2017**, *17*, 5012. DOI: 10.1021/acs.nanolett.7b02212
Featured in Caltech News and Phys.org
17. J.-J. Zhou and **M. Bernardi**
Ab initio electron mobility and polar phonon scattering in GaAs.
Physical Review B **2016**, *94*, 201201(R). DOI: 10.1103/PhysRevB.94.201201
18. **M. Bernardi**
First-principles dynamics of electrons and phonons.
European Journal of Physics B **2016**, *89*, 239. DOI: 10.1140/epjb/e2016-70399-4
19. **M. Bernardi**, J. Mustafa, J. B. Neaton, and S. G. Louie
Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals.
Nature Communications **2015**, *6*, 7044. DOI: 10.1038/ncomms8044
20. M. Palummo*, **M. Bernardi***, and J. C. Grossman
Exciton radiative lifetimes in two-dimensional transition metal dichalcogenides.
Nano Letters **2015**, *15*, 2794. *Equal contributors. DOI: 10.1021/nl503799t
21. **M. Bernardi**, D. Vigil-Fowler, J. Lischner, J. B. Neaton, and S. G. Louie
Ab initio study of hot carriers in the first picosecond after sunlight absorption in silicon.
Physical Review Letters **2014**, *112*, 257402. DOI: 10.1103/PhysRevLett.112.257402
Featured in Berkeley Lab News
22. **M. Bernardi**, M. Palummo, and J. C. Grossman
Extraordinary sunlight absorption and 1 nm-thick photovoltaics using 2D monolayer materials.
Nano Letters **2013**, *13*, 3664. (>2,500 citations). DOI: 10.1021/nl401544y
Featured in MIT News.

Invited Talks

Selected invited talks for the last 10 years:

- **2027 11th Time-Dependent Density Functional Theory Workshop**, Benasque, Spain.
  First-Principles Quantum Dynamics Toolbox for Quantum Materials.
- **2027 Workshop: Collective Excitations and Emergent Quasiparticles**, TU Munich, Germany.
  First-Principles Quantum Dynamics Toolbox for Quantum Materials.
- **2027 Electrical and Computer Engineering Colloquium**, University of California Riverside.
  Compressing Quantum Interactions in Materials: from Tensor Learning to Diagrammatics.
- **2026 UCLA Physical Chemistry Seminar**, University of California Los Angeles (UCLA).
  Compressing Quantum Interactions in Materials: from Tensor Learning to Diagrammatics.
- **2026 The 27th Asian Workshop on First-Principles Electronic Structure Calculations. (Plenary talk).** Kaohsiung, Taiwan
  Compressing Quantum Interactions in Materials: from Tensor Learning to Diagrammatics.
- **2026 National Taiwan University and IAMS Academia Sinica, Physics Department Colloquium.** Taipei, Taiwan
  First-Principles Quantum Dynamics Toolbox for Quantum Materials.
- **2026 AI4X Accelerate Conference**. National University of Singapore.
  Quantum Interactions in Materials: a New Frontier for AI.
- **2026 Workshop on Soft Matter enabled Quantum Materials**. Cornell University, Ithaca, NY.
  Compressing Quantum Interactions: Opportunities for Complex Quantum Materials.
- **2026 Condensed Matter Seminar at UC San Diego**. San Diego, CA.
  Compressing Quantum Interactions in Condensed Matter via Decomposition and Tensor Learning.
- **2026 CECAM Workshop: Quantum Materials In and Out of Equilibrium**. Bremen, Germany.
  Quantum Interactions in Materials: Compression, Diagrammatics, and Strong Coupling.
- **2025 Psi-K Workshop: First-Principles Modeling of Electron-Phonon Interactions**.
  EPFL, Lausanne, Switzerland.
  New Directions in Electron-Phonon Calculations: Compression, Diagrammatics, and Correlations.
- **2025 Caltech & University of Chicago Conference on AI+Science**. Caltech, Pasadena, CA.
  Quantum Interactions in Materials: a New Frontier for AI.
- **2025 MRS Fall Meeting**. Boston, MA.
  Polaron Transport in Complex Oxides from Novel Many-Body Calculations.
- **2025 6th Berkeley Excited State Conference**. Berkeley, CA.
  Addressing quantum interactions in materials: compression, diagrammatics, and strong coupling.
- **2025 Princeton Center for Theoretical Science Workshop: Nonadiabatic Dynamics, Electron-Phonon Interactions, and Spin-Phonon Couplings**. Princeton, NJ.
  New Directions in Electron-Phonon Calculations: Spin Dynamics, Strong Coupling, and Compression.
- **2025 DPG Meeting of the Condensed Matter Section**. Regensburg, Germany.
  Spin-Phonon and Magnon-Phonon Interactions from First Principles.
- **2025 APS March Meeting**. Anaheim, CA.
  First-Principles Exciton-Phonon and Magnon-Phonon Interactions.
- **2025 Greater Boston Theoretical Chemistry Seminar**. MIT, Cambridge, MA.
  Building the Computational Toolbox for Quantum Materials:
  Precise First-Principles Calculations of Electron and Spin Dynamics.

- **2025 Kavli Institute for Theoretical Physics Conference: Harnessing Quantum-Optical Techniques in Solid-State Materials**. KITP, Santa Barbara, CA.
  Electron-Phonon Interactions in the Strong Coupling Limit. Recorded talk is available on YouTube.
- **2025 Workshop: Quantum Thermodynamics Meets Quantum Computation**.
  Scuola Normale Superiore, Pisa, Italy.
  Quantum Circuit Simulations and Quantum Period Finding Using Reduced Density Matrices.
- **2024 Psi-K Workshop: Electronic Structure Simulations for Large-Scale Facilities**.
  EPFL, Lausanne, Switzerland.
  New Directions in Electron-Phonon Calculations.
- **2024 Physics Colloquium**. University of Pisa, Italy.
  Precise Calculations of Electron and Phonon Dynamics.
- **2024 NEST Nano Colloquium**. NEST National Laboratory, Pisa, Italy.
  Precise First-Principles Calculations of Electron and Spin Dynamics.
- **2024 MRS Spring Meeting**. Seattle, WA.
  Precise Calculations of Strong Electronic Interactions and Transport in Oxides.
- **2024 GraFOx Seminar at Paul Drude Institute**. Berlin, Germany.
  Building the Computational Toolbox for Quantum Materials:
  Precise First-Principles Calculations of Electron and Spin Dynamics.
- **2023 Materials Science and Engineering Colloquium**. Columbia University, New York.
  Building the Computational Toolbox for Quantum Materials:
  Precise First-Principles Calculations of Electron and Spin Dynamics.
- **2023 35^{th} Annual Workshop on Recent Developments in Electronic Structure Methods**.
  Merced, CA.
  Advances in Electron-Phonon Interactions and Spin Dynamics from First Principles.
- **2023 Quantum Foundry Seminar**. UC Santa Barbara, CA.
  Precise First-Principles Calculations of Electron and Spin Dynamics:
  Building the Toolbox for Quantum Materials.
- **2023 Sanibel Symposium: Spin Workshop**. University of Florida, FL.
  Theory and First-Principles Calculations of Spin-Phonon Interactions and Spin Relaxation.
- **2023 2nd Quantum Matters in Materials Science Workshop**. NIST (virtual).
  Advances in First-Principles Calculations of Electron and Spin Dynamics in Quantum Materials.
- **2023 APS March Meeting**. Las Vegas, NV.
  Theory and First-Principles Calculations of Spin-Phonon Interactions and Spin Relaxation.
- **2023 5th Functional Oxide Thin Films Conference**. Cancun, Mexico.
  First-Principles Calculations of Strong Electronic Interactions in Complex Oxides.
- **2022 Vienna Quantum Seminar Lecture**. Vienna, Austria.
  Precise and Parsimonious Computational Quantum Physics: From Electrons in Materials to Quantum Circuits.
- **2022 The 23rd Asian Workshop on First-Principles Electronic Structure Calculations (Plenary Talk)**. Virtual.
  Frontiers of First-Principles Electron-Phonon Interactions: Weak-to-Strong, Correlated, Spinful, and Data-Driven.
- **2022 Workshop on First-Principles Modeling of Defects in Solids**. ETH Zurich, Switzerland.

Predicting Electronic Interactions and Transport Governed by Polarons and Defects.

- **2022 ICTP Workshop on Thermal Transport**. Virtual.
  Advances in Computing Electron Interactions and Dynamics from First Principles.
- **2022 IPAM Workshop on Model Reduction in Quantum Mechanics**. Los Angeles CA, USA.
  Precise Calculations of Electron Interactions and Dynamics in Condensed Matter.
- **2022 MRS Spring Meeting**. Honolulu, HI.
  Nonequilibrium Dynamics of Interacting Electrons, Phonons and Excitons from First Principles.
- **2022 ACS Spring Meeting**. San Diego, CA.
  Precise First-Principles Tools for Electron Dynamics in Quantum Materials.
- **2021 Harvard Quantum Materials and Devices Seminar**. Harvard, Cambridge MA (virtual).
  Novel Computational Tools for Electron Dynamics in Quantum Materials.
- **2021 MRS Spring Meeting**. Virtual.
  Understanding Charge Transport in Transition Metal Oxides with Novel First-Principles Computational Methods.
- **2021 APS March Meeting**. Virtual.
  Ultrafast Dynamics of Coupled Electrons, Phonons and Excitons from First Principles.
- **2021 Photon Science Seminar, SLAC / Stanford**. Virtual.
  Ultrafast Dynamics of Coupled Electrons, Phonons and Excitons from First Principles.
- **2021 Berkeley Excited States Conference, UC Berkeley**. Virtual.
  Ultrafast Dynamics of Coupled Electrons, Phonons and Excitons from First Principles.
- **2020 Psi-K Workshop on Electron-Phonon Interactions**. San Sebastian, Spain (virtual).
  Ab Initio Electron-Phonon Interactions and Charge Transport – from Weak to Strong Coupling.
- **2020 ICTP Workshop: Excited Charge Dynamics in Semiconductors**. Trieste, Italy (virtual).
  Ultrafast Dynamics of Coupled Electrons, Phonons and Excitons from First Principles.
- **2020 University of Illinois at Chicago, Physics Colloquium.** Chicago, IL (virtual).
  Electron Dynamics in Materials from First Principles.
- **2020 University of Illinois Urbana-Champaign, Materials Science Seminar.** Urbana, IL.
  Electron Dynamics in Materials from First Principles.
- **2020 Arizona State University, Materials Science Colloquium.** Phoenix, AZ (virtual).
  Electron Dynamics in Materials from First Principles.
- **2020 U.S. Kavli Frontiers of Science Symposium of the National Academy of Sciences**.
  Poster presentation (virtual).
- **2020 APS March Meeting**. Denver, CO (virtual).
  Toward Precise First-Principles Simulations of the Ultrafast Dynamics of Electrons and Phonons.
- **2020 TMS Meeting**. San Diego, CA.
  Advances in Computing Electron Dynamics in Materials from First Principles.
- **2019 NanoGe Fall Meeting.** Berlin, Germany.
  Advances in Computing Electron Dynamics in Perovskite Materials from First Principles.
- **2019 QuTech Seminar, TU Delft.** Delft, Netherlands.
  Electron Dynamics in Materials from First Principles.
- **2019 CCQ Flatiron Institute of the Simons Foundation.** New York, NY.
  Advances in Computing Electron Dynamics in Materials from First Principles.

- **2019 Psi-K Workshop: Ultrafast Physics from Molecules to Nanostructures.**
  San Sebastian, Spain.
  Advances in Computing Ultrafast Dynamics of Electrons, Phonons and Excitons from First Principles.
- **2019 University of Maryland, Physics Department Colloquium.** Baltimore, MD.
  Electron Dynamics in Materials from First Principles.
- **2019 ACS Spring Meeting.** Orlando, FL.
  Talk 1: Advances in Computing Charge Carrier Dynamics from First Principles.
  Talk 2: Light-Matter Interaction in Two-Dimensional Transition Metal Dichalcogenides.
- **2019 4th Functional Oxide Thin Films Conference.** Torres Vedras, Portugal.
  Advances in Computing Charge Carrier Dynamics in Oxides from First Principles.
- **2019 UC Davis Chemistry Department Colloquium** Davis, CA.
  Charge Carrier Dynamics in Materials from First Principles.
- **2018 Cal State Los Angeles Physics Department Colloquium** Los Angeles, CA.
  Charge Carrier Dynamics in Materials from First Principles.
- **2018 UC Riverside Mechanical Engineering Department Colloquium**. Riverside, CA.
  Advances in Computing Charge Carrier Dynamics from First Principles.
- **2018 APS March Meeting**. Los Angeles, CA.
  Talk 1: Advances in Computing Charge Transport and Hot Carrier Dynamics from First Principles.
  Talk 2: APS Tutorial: Electron-Phonon Interactions from First Principles.
- **2017 TMS Meeting**. San Diego, CA.
  Talk 1: Light-Matter Interaction in Two-Dimensional Transition Metal Dichalcogenides.
  Talk 2: Recent Advances in Electron-Phonon Calculations: Theory, Computation, and Applications.
- **2017 World Association of Theoretical and Computational Chemistry**. Munich, Germany.
  Advances in Computing Charge Carrier Dynamics from First Principles.
- **2017 UC Merced Physics Department Colloquium**. Merced, CA.
  Advances in Computing Charge Carrier Dynamics from First Principles.
- **2017 EPFL Materials Science Department Colloquium**. Lausanne, Switzerland.
  Ab Initio Electron-Phonon Calculations: Theory, Computation, and Application to Carrier Dynamics.
- **2017 Trinity College, Physics Department**. Dublin, Ireland.
  Ab Initio Electron-Phonon Calculations: Theory, Computation, and Application to Carrier Dynamics.
- **2017 Cambridge University, Physics Department**. Cambridge, UK.
  Charge Carrier Dynamics and Light Emission in Materials from First Principles.
- **2016 Biennial Total Energy and Force Methods Workshop**. University of Luxembourg.
  Ultrafast Dynamics of Excited Electrons in Materials.
- **2016 Hume-Rothery Award Symposium, TMS Annual Conference**. Nashville, TN.
  Ultrafast Dynamics of Excited Electrons in Materials.