MARCO BERNARDI

CONTACT INFORMATION

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ADDRESS

California Institute of Technology
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RESEARCH INTERESTS

- Materials physics, electronic structure theory, computational physics
- Interactions, transport, and nonequilibrium dynamics in conventional and quantum materials
- Materials for electronics, energy, and quantum technologies

EDUCATION

- **Massachusetts Institute of Technology**, Cambridge, MA, USA
  Ph.D. in Materials Science, June 2013. Advisor: Prof. Jeffrey C. Grossman
- **University of Rome Tor Vergata**, Rome, Italy
  M.Sc. (Laurea Specialistica) in Materials Science, January 2008. *Summa Cum Laude*
- **University of Rome La Sapienza**, Rome, Italy
  B.Sc. (Laurea Triennale) in Chemistry, November 2004. *Summa Cum Laude*

RESEARCH AND PROFESSIONAL EXPERIENCE

- **Professor**
  Department of Applied Physics and Materials Science, and Department of Physics
  California Institute of Technology. Pasadena, CA, USA
  Dates: June 2021 –
  Leads a research group focused on understanding quantum interactions and dynamics in materials
- **Assistant Professor**
  Department of Applied Physics and Materials Science
  California Institute of Technology. Pasadena, CA, USA
  Dates: September 2015 – May 2021
- **Post-Doctoral Fellow**
  Physics Department, University of California, Berkeley and
  Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA
  Dates: September 2013 – August 2015
  Supervisors: Prof. Steven G. Louie, Prof. Jeffrey B. Neaton
  Developed new first-principles methods for electron dynamics in materials
- **Research Assistant**
  Massachusetts Institute of Technology, Cambridge, MA, USA
  Department of Materials Science and Engineering
  Dates: September 2008 – August 2013
  Supervisor: Prof. Jeffrey C. Grossman
  Studied novel materials and physical processes for solar energy conversion

HONORS AND AWARDS

- 2020 ISSNAF "Franco Strazzabosco" Young Investigator Award
- 2019 Emerging Young Investigator Award at the 4th Functional Oxide Thin Films Conference
- 2018 NSF CAREER Award
- 2017 Air Force Young Investigator 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

TEACHING

- Structure and Bonding in Materials (MS 131). Taught from 2016 to 2025
- Introduction to Computational Methods for Science and Engineering (MS 141). Taught from 2020 to 2025
- Computational Solid State Physics and Materials Science (APh 256). Taught in 2018

CURRENT GROUP MEMBERS

Graduate students
Applied Physics: Yao Luo, David Abramovitch. *Materials Science*: Sergei Kliavinek.
Physics: Jia (Kelly) Yao, Ina Sorensen. *Chemistry*: Khoa Le, Laurie Tan

Postdocs
Shiyu Peng, Tommaso Chiarotti

PROFESSIONAL ACTIVITIES AND AFFILIATIONS

- **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 (among others).
- **Memberships**: American Physical Society, American Chemical Society, Materials Research Society.
- **Organizer:** Organized invited symposia on ultrafast dynamics at APS March Meetings from 2020 to 2025.
- **Consulting:** Reviewed high-performance computing proposals for ALCC in the US and PRACE in Europe.
- **Editor:** Section editor for the 2019 Handbook of Materials Modeling (Springer).

RECENT INVITED TALKS

- **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.
- **2025 Workshop: Quantum Thermodynamics Meets Quantum Computation**. SNS, 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, 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, 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$^{\text{th}}$ 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, USA (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.

PUBLICATIONS

Metrics – h-index: 40 Citations: 10,000 (see Google Scholar)
$\sim$80 peer reviewed papers. For the full publication list, see the group website

Selected Publications
(see the magenta links for press articles)

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
   See the press articles from Caltech News and Physics World.

2. 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
   See the press article from Caltech News

3. 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

4. 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.
   Physical Review Materials **2023** *7*, 093801 (Editor's Suggestion). DOI: 10.1103/PhysRevMaterials.7.093801

5. 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
   See the press article from Caltech News

6. 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
   See the press article from EPFL

7. 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
   See the press article in the Caltech News
   The code can be downloaded at https://perturbo-code.github.io/

8. 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

9. 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

10. 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

11. 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
See the press article in the Caltech News

12. 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
See the press article in the Caltech News

13. K. Frohna, T. Deshpande, J. Harter, B. Barker, J. B. 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
See the press article in the Caltech News

14. 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
See the press articles in the Caltech News and phys.org

15. J.-J. Zhou and **M. Bernardi**
Ab Initio Electron Mobility and Polar Phonon Scattering in GaAs.
Physical Review B (Rapid Communication) **2016**, *94*, 201201. DOI: 10.1103/PhysRevB.94.201201

16. **M. Bernardi**
First-Principles Dynamics of Electrons and Phonons.
European Journal of Physics B **2016**, *89*, 239. DOI: 10.1140/epjb/e2016-70399-4

17. **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

18. 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

19. **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
See the press article in the Berkeley Lab News

20. **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. DOI: 10.1021/nl401544y
See the press articles in MIT News and NERSC. Cited over 2000 times.