MARCO BERNARDI

CONTACT INFORMATION

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ADDRESS

California Institute of Technology
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RESEARCH INTERESTS

- Computational materials physics, electronic structure theory
- Electron interactions, transport, and nonequilibrium dynamics in 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 electron 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 every year from 2016 to 2023
- Introduction to Computational Methods for Science and Engineering (MS 141). Taught from 2020 to 2023
- Computational Solid State Physics and Materials Science (APh 256). Taught in 2018

CURRENT GROUP MEMBERS

Graduate students
Applied Physics: Benjamin Chang, Dhruv Desai, Yao Luo, David Abramovitch, Shaelyn Iyer.
Materials Science: Sergei Kliavinek. *Physics*: Jia (Kelly) Yao, Ina Sorensen. *Chemistry*: Khoa Le

Postdocs
Shiyu Peng

PROFESSIONAL ACTIVITIES AND AFFILIATIONS

- **Reviewer**: Nature, Science, Nature Materials, Nature Physics, Nature Nanotechnology, Nature Communications, Science Advances, Physical Review Letters, Physical Review X, Physical Review B, Physical Review Materials, Nano Letters, Materials Today Physics, Journal of Physical Chemistry Letters (among others).
- **Memberships**: American Physical Society, American Chemical Society, Materials Research Society.
- **Editor:** Section editor for the 2019 Handbook of Materials Modeling (Springer).
- **Organizer:** Organized invited symposia on ultrafast dynamics in the 2020, 2021, and 2024 APS March Meetings.
- **Consulting:** Reviewed high-performance computing proposals for ALCC in the US and PRACE in Europe.

RECENT INVITED TALKS

- **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.
- **2023 SIAM Conference on Computational Science and Engineering**. Amsterdam, Netherlands.
  Nonequilibrium Dynamics of Interacting Electrons, Phonons and Excitons from First Principles.
- **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 ETH Zurich Workshop on First-Principles Modeling of Defects in Solids**. 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 Quantum Mechanical Calculations of Electron Interactions and Dynamics in Condensed Matter.
- **2022 MRS Spring Meeting**. Honolulu HI, USA.
  Nonequilibrium Dynamics of Interacting Electrons, Phonons and Excitons from First Principles.
- **2022 ACS Spring Meeting**. San Diego CA, USA.
  Precise First-Principles Tools for Electron Dynamics in Quantum Materials.
- **2021 Quantum Materials and Devices Seminar, Harvard**. 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.

PUBLICATIONS

Metrics – h-index: 37 Citations: 7,500 (see Google Scholar)
Total of 67 peer reviewed publications. For the full publication list, see the group website

Selected Publications
(see the magenta links for press articles)

1. 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

2. 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

3. 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

4. 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/

5. 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

6. 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

7. 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

8. 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

9. I.-T. Lu, J.-J. Zhou, and **M. Bernardi**
   Efficient Ab Initio Calculations of Electron-Defect Scattering and Defect-Limited Carrier Mobility.
   Physical Review Materials **2019**, *3*, 033804 (Editor's Suggestion). DOI: 10.1103/PhysRevMaterials.3.033804

10. 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

11. 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

12. N.-E. Lee, J.-J. Zhou, L. Agapito and **M. Bernardi**
Charge Transport in Organic Molecular Semiconductors from First Principles:
The Band-Like Hole Mobility in a Naphthalene Crystal.
Physical Review B **2018**, *97*, 115203. DOI: 10.1103/PhysRevB.97.115203

13. 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

14. 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

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

16. **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

17. 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

18. **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 feature articles in the Berkeley Lab News

19. **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 by the MIT News and NERSC. Cited over 1800 times.

20. **M. Bernardi**, N. Ferralis, J. H. Wan, R. Villalon, and J. C. Grossman
Solar Energy Generation in Three Dimensions.
Energy and Environmental Science **2012**, *5*, 6880. DOI: 10.1039/c2ee21170j
See the press articles in the the MIT News and Technology Review. Featured in the Wired magazine