MARCO BERNARDI

CONTACT INFORMATION

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ADDRESS

California Institute of Technology
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MAIN RESEARCH INTERESTS

- First-principles computation of electronic and optical properties of materials
- Ultrafast electron and excited state dynamics in materials
- Transport of charge carriers, spin, excitons and phonons
- Novel materials and interfaces for electronics, optoelectronics and solar energy

EDUCATION

- **Massachusetts Institute of Technology**, Cambridge, MA, USA
  Ph.D. in Materials Science, June 2013. GPA 5.0. 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. Major in Materials Chemistry. *Summa Cum Laude*.

RESEARCH AND PROFESSIONAL EXPERIENCE

- **Assistant Professor**
  Department of Applied Physics and Materials Science
  California Institute of Technology. Pasadena, CA, USA
  Dates: September 2015 – Present

- **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
  Carried out research on ab initio charge carrier dynamics in semiconductors and metals.

- **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
  Carried out research on novel materials and physical processes for solar energy conversion.

HONORS AND AWARDS

- 2018 NSF CAREER Award
- 2017 AFOSR Young Investigator Award
- 2015 Psi-K Volker Heine Young Investigator Award
- 2011 Intel Ph.D. Fellowship
- 2009 Graduate Student Exceptional Performance Award
- 2007 Australian Endeavour Research Fellowship

TEACHING

- Structure and Bonding in Materials (MS 131). Taught in Winter 2016, Fall 2016, Fall 2017.
- Computational Solid State Physics and Materials Science (APh 256). Taught in Spring 2018.
- Materials Research Lectures (MS 110A). Instructor in charge of organizing the department seminars for Fall 2017 through Fall 2018.

GRADUATE STUDENT ADVISEES

Materials Science: I-Te Lu, Megan Schill, Xiao Tong
Applied Physics: Vatsal Jhalani, Austin Liu, Jinsoo Park
Physics: Nien-En Lee, Hsiao-Yi Chen

POSTDOCTORAL ADVISEES

Jin-Jian Zhou, Raffaello Bianco

CALTECH SERVICE

- Graduate student admission committee, both in Applied Physics and Materials Science (every year since 2015)
- Faculty search committee in Materials Science (2017−2018)
- Served on roughly 10 candidacy exams and thesis defenses, both in Applied Physics and Materials Science
- Resnick Institute postdoctoral fellowship − reviewed applications (Fall 2016).
- Organized the Materials Science department weekly seminars (Fall 2017 − Winter 2019)

PROFESSIONAL ACTIVITIES AND AFFILIATIONS

- **Reviewer**: Science, Nature Nanotechnology, Nature Materials, Nature Physics, Nature Communications, Science Advances, Scientific Reports, Physical Review Letters, Physical Review B, Applied Physics Letters, Nano Letters, ACS Nano, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, Nanotechnology, Nanoscale, Applied Surface Science (among others).
- **Memberships**: American Physical Society (APS), American Chemical Society (ACS), Materials Research Society (MRS), and The Minerals, Metals & Materials Society (TMS).
- **Editor**: Editor of the photovoltaics section of the 2019 Handbook of Materials Modeling (Springer).
- **Consulting:** Reviewed grants for the MIT Energy Initiative. Reviewed proposals for supercomputing time for the Partnership for Advanced Computing in Europe (PRACE).

INVITED TALKS

Note: 2019 talks are accepted invitations.

- **2019 Spring ACS Meeting.** Orlando FL, USA.
- **2019 NanoGe Fall Meeting.** Berlin, Germany.
- **2019 UC Davis Chemistry Department Colloquium** Davis CA, USA.
- **2018 International Conference on Non-equilibrium Dynamics in the Time Domain**. Kerkrade, Netherlands. Advances in Computing Ultrafast Carrier and Exciton Dynamics from First Principles.
- **2018 UC Riverside Mechanical Engineering Department Colloquium**. Riverside CA, USA. Advances in Computing Charge Carrier Dynamics from First Principles.
- **2018 Theory Symposium of the Max Planck Society**. Berlin, Germany. Charge Carrier Dynamics from First Principles.
- **2018 APS March Meeting**. Los Angeles CA, USA. Invited talk: Advances in Computing Charge Transport and Hot Carrier Dynamics from First Principles. Tutorial: Electron-Phonon Interactions from First Principles.

- **2017 World Association of Theoretical and Computational Chemistry (WATOC)**. Munich, Germany.
  Advances in Computing Charge Carrier Dynamics from First Principles.
- **2017 UC Merced Physics Department Colloquium**. Merced CA, USA.
  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 Keck Energy Materials Research Workshop**. California State University, Long Beach CA.
  New Frontiers in Solar Cell Materials: Ultrathin, Ultrafast, and Complex.
- **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, USA.
  Ultrafast Dynamics of Excited Electrons in Materials.
- **2015 Oxford Materials Modeling Laboratory Seminar**. Oxford, UK.
  Ultrafast Dynamics of Excited Electrons in Materials for Energy Applications.
- **2015 Thomas Young Center Soiree on Photovoltaics at Imperial College**. London, UK.
  New Regimes for Solar Cell Materials: Ultrafast, Ultrathin, and Complex.
- **2015 Center for Free Electron Laser (CFEL) Theory Seminar**. Hamburg, Germany.
  Ultrafast Dynamics of Excited Electrons in Materials for Energy Applications.
- **2015 Psi-K Conference (Volker Heine Young Investigator Award Symposium)**. San Sebastian, Spain.
  Ultrafast Dynamics of Excited Electrons in Materials for Energy Applications.
- **2015 27th Workshop on Recent Development in Electronic Structure Theory**. Seattle WA, USA.
  Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications.
- **2015 Stanford Materials Science Colloquium**. Stanford CA, USA.
  Ultrafast Dynamics of Excited Electrons in Semiconductors and Metals for Energy Applications.
- **2014 International Conference on the Physics of Semiconductors**. Austin TX, USA.
  Hot Carriers in the First Picosecond After Sunlight Absorption in Silicon and GaAs from First-Principles.
- **2014 Caltech / HKUST Workshop on Fuel Cells and Electrolyzers**. Hong Kong.
  Ultrafast Processes and Ultrathin Materials in Solar Energy Conversion.
- **2014 Technical University Federico Santa Maria − Physics Colloquium**. Valparaiso, Chile.
  Ultrafast Processes and Ultrathin Materials in Solar Energy Conversion.
- **2013 APS March Meeting**. Baltimore MD, USA.
  Computational Spectroscopy for Nanoscale Photovoltaics.
- **2013 Caltech Materials Science Department Colloquium**. Pasadena CA, USA.
  Novel Materials, Theoretical Spectroscopy, and Multiscale Simulation in Nanoscale Photovoltaics.

PUBLICATION LIST (PEER REVIEWED ARTICLES)

See also my Google Scholar profile
See the magenta links below for press articles about my research

32. J.-J. Zhou, O. Hellman and **M. Bernardi**
Temperature Dependent Electron-Phonon Scattering and Electron Mobility in $SrTiO_3$ Perovskite from First Principles. *Submitted*.
Preprint: arXiv 1806.05775

31. L. Agapito, **M. Bernardi**
Ab Initio Electron-Phonon Interactions Using Atomic Orbital Wavefunctions.
Physical Review B **2018**, *97*, 235146. DOI: 10.1103/PhysRevB.97.235146

30. H.-Y. Chen, M. Palummo, D. Sangalli and **M. Bernardi**
Theory and Ab Initio Computation of the Anisotropic Light Emission in Monolayer Transition Metal Dichalcogenides.
Nano Letters **2018**, *18*, 3839. DOI: 10.1021/acs.nanolett.8b01114

29. 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

28. 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

27. 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

26. E. Najafi, V. Ivanov, A. Zewail and **M. Bernardi**
Super-Diffusion of Excited Carriers in Semiconductors.
Nature Communications **2017** *8*, 15177. DOI: 10.1038/ncomms15177
See the press article in the Caltech News and phys.org

25. I.-T. Lu and **M. Bernardi**
Using Defects to Store Energy in Materials – a Computational Study.
Scientific Reports **2017**, *7*, 3403. DOI: 10.1038/s41598-017-01434-8

24. 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

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

22. **M. Bernardi** and J.C. Grossman
Computer Calculations across Time and Length Scales in Photovoltaics.
Energy and Environmental Science **2016**, *9*, 2197. DOI: 10.1039/C6EE01010E

21. J. Mustafa*, **M. Bernardi***, J. B. Neaton, and S. G. Louie
Ab Initio Electronic Relaxation Times and Transport in Noble Metals.
Physical Review B **2016**, *94*, 155105. (*Equal Contributors). DOI: 10.1103/PhysRevB.94.155105

20. **M. Bernardi**, M. Palummo, C. Ataca, and J. C. Grossman
Optical and Electronic Properties of Two-Dimensional Layered Materials.
Nanophotonics **2016**, *6*, 111. DOI: 10.1515/nanoph-2015-0030

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

18. **M. Bernardi**, D. Vigil-Fowler, C. S. Ong, J. B. Neaton, and S. G. Louie
Ab Initio Study of Hot Electrons in GaAs.
Proc. Natl. Acad. Sci. USA **2015**, *112*, 5291. DOI: 10.1073/pnas.1419446112

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

16. **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 articles in the Berkeley Lab News and DOE−BES highlights

15. F. Risplendi, **M. Bernardi**, G. Cicero, and J. C. Grossman
Structure-Property Relations in Amorphous Carbon for Photovoltaics.
Applied Physics Letters **2014**, *105*, 043903. DOI: 10.1063/1.4891498

14. M. Gong, T. A. Shastry, Y. Xie, **M. Bernardi**, D. Jasion, T. J. Marks, J. C. Grossman, S. Ren, and M. Hersam
Polychiral Semiconducting Carbon Nanotube-Fullerene Solar Cells.
Nano Letters **2014**, *14*, 5308. DOI: 10.1021/nl5027452
See the press article by Physics World

13. A. El Ballouli, E. Alarousu, **M. Bernardi**, S. Aly, A. LaGrow, O. Bakr, and O. Mohammed
Tunable Ultrafast Charge Transfer at the PbS Quantum Dot and PCBM Interface.
J. Am. Chem. Soc. **2014**, *136*, 6952. Cover article in JACS. DOI: 10.1021/ja413254g

12. **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 800 times.

11. **M. Bernardi** and J. C. Grossman
Optimal Sunlight Harvesting in Photovoltaics and Photosynthesis.
J. Phys. Chem. C **2013**, *117*, 26896. DOI: 10.1021/jp4090348

10. P. V. Kumar, **M. Bernardi**, and J. C. Grossman
The Impact of Functionalization on the Stability, Work Function and Photoluminescence of Graphene Oxide.
ACS Nano **2013**, *7*, 1638. DOI: 10.1021/nn305507p

9. **M. Bernardi**, M. Palummo, and J. C. Grossman
Semiconducting Monolayer Materials as a Tunable Platform for Excitonic Solar Cells.
ACS Nano **2012**, *6*, 10082. DOI: 10.1021/nn303815z

8. **M. Bernardi**, J. Lohrman, P. Kumar, A. Kirkeminde, N. Ferralis, J. C. Grossman, and S. Ren
Nanocarbon-Based Photovoltaics.
ACS Nano **2012**, *6*, 8896. DOI: 10.1021/nn302893p
See the press article in Scientific American and Nanowerk

7. **M. Bernardi**, M. Palummo, and J. C. Grossman
Optoelectronic Properties and Excitons in Hybridized Boron Nitride and Graphene Hexagonal Monolayers.
Physical Review Letters **2012**, *108*, 226805. DOI: 10.1103/PhysRevLett.108.226805

6. **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.
Also featured in the Wired magazine and tens of media outlets.

5. S. Ren*, **M. Bernardi***, R.R. Lunt, V. Bulovic, J. C. Grossman, and S. Gradecak
Efficient Carbon Nanotube / P3HT Solar Cells: Active Layer Morphology, Electrical and Optical Properties.
Nano Letters **2011**, *11*, 5316. *Equal Contributors. DOI: 10.1021/nl202796u

4. **M. Bernardi**, M. Giulianini, and J. C. Grossman
Self-Assembly and Its Impact on Interfacial Charge Transfer in Carbon Nanotube / P3HT Solar Cells.
ACS Nano **2010**, *4*, 6599. DOI: 10.1021/nn1018297

3. B. Myers, **M. Bernardi**, and J. C. Grossman
Three-Dimensional Photovoltaics.
Applied Physics Letters **2010**, *96*, 071902. DOI: 10.1063/1.3308490

2. L. Persichetti, A. Sgarlata, M. Fanfoni, **M. Bernardi**, and A. Balzarotti
Step-step Interaction on Vicinal Si (001) Surfaces Studied by Scanning Tunneling Microscopy.
Physical Review B **2009**, *80*, 075315. DOI: 10.1103/PhysRevB.80.075315

1. **M. Bernardi**, A. Sgarlata, M. Fanfoni, A. Balzarotti and N. Motta
A Study of the Pair Distribution Function of Self-Organized Ge Quantum Dots.
Applied Physics Letters **2008**, *93*, 031917. DOI: 10.1063/1.2965122