CURRICULUM VITAE: MARCO BERNARDI

CONTACT INFORMATION

E-mail: bmarco@caltech.edu
Phone: 626-395-2515
http://bernardi.caltech.edu

ADDRESS

California Institute of Technology
1200 E California Blvd. MC 107-81
Pasadena CA, 91125

RESEARCH INTERESTS

- Computational materials physics, first-principles electronic structure theory, condensed matter theory
- Transport and ultrafast dynamics of charge carriers, spin, phonons and excitons
- Materials for electronics, optoelectronics, 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
  Carried out research on 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
  Carried out research on novel materials and physical processes for solar energy conversion.

HONORS AND AWARDS

- 2020 ISSNAF "Franco Strazzabosco" Young Investigator Award for research in engineering
- 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 for electronic structure theory
- 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 & 2017, Winter 2019 − 2022.
- Computational Solid State Physics and Materials Science (APh 256). Taught in Spring 2018.
- Introduction to Computational Methods for Science and Engineering (MS 141). Taught in Spring 2020 − 2022.

CURRENT GRADUATE STUDENT ADVISEES

Applied Physics: Benjamin Chang, Dhruv Desai, Yao Luo, David Abramovitch
Materials Science: Shaelyn Iyer
Physics: Jia (Kelly) Yao
Chemistry: Khoa Le

CURRENT POSTDOCTORAL ADVISEES

Ivan Maliyov, Jinsoo Park

ALUMNI

Postdocs − current position:
Jin-Jian Zhou − Assistant Professor at Beijing Institute of Technology
Shiyuan Gao − Research Scientist at Johns Hopkins
Sergio Pineda Flores −
Luis Agapito − Software engineer at Synopsys Inc.
Raffaello Bianco − Postdoc at U. Basque Country

Students − current position:
Vatsal Jhalani − Postdoc at NASA JPL
Nien-En Lee − Engineer at Media Tek Inc.
I-Te Lu − Humboldt Fellow and postdoc at Max Planck in Hamburg
Hsiao-Yi Chen − Special Postdoctoral Fellow at RIKEN in Japan
Jinsoo Park − Postdoc at Caltech.

PROFESSIONAL ACTIVITIES AND AFFILIATIONS

- **Reviewer**: Science, Nature Nanotechnology, Nature Materials, Nature Physics, Nature Communications, Science Advances, Scientific Reports, Physical Review Letters, Physical Review B, Physical Review X, Physical Review Materials, Applied Physics Letters, Nano Letters, ACS Nano, Materials Today Physics, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, Nanotechnology, Nanoscale (among others).
- **Memberships**: American Physical Society (APS), American Chemical Society (ACS), Materials Research Society (MRS), and The Minerals, Metals & Materials Society (TMS).
- **Editor:** Section editor for the 2019 Handbook of Materials Modeling (Springer).
- **Organizer:** Organized invited symposia on ultrafast dynamics for the 2020 and 2021 APS March Meetings.
- **Consulting:** Reviewed proposals for the Partnership for Advanced Computing in Europe (PRACE).

INVITED TALKS

- **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.
- **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 on 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, USA (virtual).
  Electron Dynamics in Materials from First Principles.
- **2020 University of Illinois Urbana-Champaign, Materials Science Seminar.** Urbana IL, USA (virtual).
  Electron Dynamics in Materials from First Principles.
- **2020 Arizona State University, Materials Science Colloquium.** Phoenix AZ, USA (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, USA (virtual).
  Talk 1: Toward Precise First-Principles Simulations of the Ultrafast Dynamics of Electrons and Phonons.
  Talk 2 (given by my post-doc, Jin-Jian Zhou): Advances in Computing Charge Carrier Dynamics in Oxides.
- **2020 TMS Meeting (Computational Thermodynamics and Kinetics Symposium)**. San Diego CA, USA.
  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 Colloquium, TU Delft.** Delft, Netherlands.
  Electron Dynamics in Materials from First Principles.
- **2019 Flatiron Institute of the Simons Foundation.** New York City, USA.
  Advances in Computing Electron Dynamics in Materials from First Principles.
- **2019 Psi-K Workshop on Ultrafast Physics from Molecules to Nanostructures.** San Sebastian, Spain.
  Advances in Computing the Ultrafast Dynamics of Electrons, Phonons and Excitons from First Principles.

- **2019 University of Maryland, Physics Department Colloquium.** Baltimore MD, USA.
  Electron Dynamics in Materials from First Principles.
- **2019 ACS Spring Meeting.** Orlando FL, USA.
  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, USA.
  Charge Carrier Dynamics in Materials from First Principles.
- **2018 Cal State Los Angeles Physics Department Colloquium** Los Angeles CA, USA.
  Charge Carrier Dynamics in Materials from First Principles.
- **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 TMS Meeting**. San Diego CA, USA.
  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 (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 for 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)

Metrics – h-index: 32 Citations: 5,800 (see Google Scholar)
See the magenta links for press articles on our work.

58. J. Park, J.-J. Zhou, Y. Luo, **M. Bernardi**
Predicting Electron Spin Decoherence with a Many-Body First-Principles Approach.
Submitted. Preprint: arXiv 2203.06401

57. H.-Y. Chen, A. Mitridate, T. Trickle, Z. Zhang, **M. Bernardi**, K. M. Zurek
Dark Matter Direct Detection in Materials with Spin-Orbit Coupling.
Submitted. Preprint: arXiv 2202.11716

56. Y. Luo, B. K. Chang, **M. Bernardi**
Comparison of the Canonical Transformation and Energy Functional Formalisms
for Ab Initio Calculations of Self-Localized Polarons.
Physical Review B **2022** 105, 155132. DOI: 10.1103/PhysRevB.105.155132

55. B.K. Chang, J.-J. Zhou, N.-E. Lee and **M. Bernardi**
Intermediate Polaronic Charge Transport in Organic Crystals from a Many-Body First Principles Approach.
NPJ Computational Materials **2022**, 8, 63. DOI: 10.1038/s41524-022-00742-6

54. I.-T. Lu, J.-J. Zhou, J. Park and **M. Bernardi**
Ab Initio Ionized-Impurity Scattering and Charge Transport in Doped Materials.
Physical Review Materials (Letter) **2022**, 6, L010801. DOI: 10.1103/PhysRevMaterials.6.L010801

53. I. Maliyov, J. Park and **M. Bernardi**
Ab Initio Electron Dynamics in High Electric Fields: Accurate Predictions of Velocity-Field Curves.
Physical Review B (Letter) **2021**, 104, L100303. DOI: 10.1103/PhysRevB.104.L100303

52. 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.

51. N.-E. Lee, H.-Y. Chen, J.-J. Zhou and **M. Bernardi**
Facile Ab Initio Approach for Self-Localized Polarons from Canonical Transformations.
Physical Review Materials **2021**, *5*, 063805. DOI: 10.1103/PhysRevMaterials.5.063805

50. T. Truttmann, J.-J. Zhou, I-T. Lu, A. Rajapitamahuni, F. Liu, T. E. Mates, **M. Bernardi** and B. Jalan
Combined Experimental-Theoretical Study of Electron Mobility-Limiting Mechanisms in $SrSnO_3$.
Communications Physics **2021**, *4*, 241. DOI: 10.1038/s42005-021-00742-w.

49. S. Gao, H.-Y. Chen, and **M. Bernardi**
Radiative Properties of Quantum Emitters in Boron Nitride from Excited State Calculations and Bayesian Analysis.
npj Computational Materials **2021**, *7*, 85. DOI: 10.1038/s41524-021-00544-2

48. X. Tong and **M. Bernardi**
Toward Precise Simulations of the Coupled Ultrafast Dynamics of Electrons and Atomic Vibrations in Materials.
Physical Review Research **2021**, *3*, 023072. DOI: 10.1103/PhysRevResearch.3.023072

47. D. Desai, B. Zviazhynski, J.-J. Zhou and **M. Bernardi**
Magnetotransport in Semiconductors and Two-Dimensional Materials from First Principles.
Physical Review B (Letter) **2021**, *103*, L161103 (Editor's Suggestion). DOI: 10.1103/PhysRevB.103.L161103

46. 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
The code can be downloaded at http://perturbo.caltech.edu
See the press article in the Caltech News.

45. 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

44. J. Park, J.-J. Zhou, V. Jhalani, C. E. Dreyer, and **M. Bernardi**
Long-Range Quadrupole Electron-Phonon Interaction from First Principles.
Physical Review B **2020**, *102*, 125203. DOI: 10.1103/PhysRevB.102.125203

43. 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

42. **M. Bernardi**
Physical Origin of the One-Quarter Exact Exchange in Density Functional Theory.
J. Phys.: Condens. Matter **2020**, *32*, 385501. DOI: 10.1088/1361-648x/ab9409

41. N.-E. Lee, J.-J. Zhou, H.-Y. Chen, and **M. Bernardi**
Ab Initio Electron-Two-Phonon Scattering in GaAs from Next-to-Leading Order Perturbation Theory.
Nature Communications **2020**, *11*, 1607. DOI: 10.1038/s41467-020-15339-0

40. I.-T. Lu, J. Park, J.-J. Zhou, and **M. Bernardi**
Ab Initio Electron-Defect Interactions using Wannier Functions.
npj Computational Materials **2020**, *6*, 17. DOI: 10.1038/s41524-020-0284-y

39. 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

38. 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.

37. V. A. Jhalani, H.-Y. Chen, M. Palummo, and **M. Bernardi**
Precise Radiative Lifetimes in Bulk Crystals from First Principles: The Case of Wurtzite GaN.
J. Phys.: Condens. Matter **2019**, *32*, 084001. DOI: 10.1088/1361-648x/ab5563
Part of the 2019 Emerging Leaders in Condensed Matter.

36. H.-Y. Chen, V. A. Jhalani, M. Palummo, **M. Bernardi**
Ab Initio Calculations of Exciton Radiative Lifetimes in Bulk Crystals, Nanostructures and Molecules.
Physical Review B **2019**, *100*, 075135. DOI: 10.1103/PhysRevB.100.075135

35. 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

34. A. J. Martinolich, C.-W. Lee, I-T. Lu, S. Bevilacqua, M. Preefer, **M. Bernardi**, A. Schleife and K. See
Solid-State Divalent Ion Conduction in $ZnPS_3$
Chem. Mater. **2019**, *31*, 3652. DOI: 10.1021/acs.chemmater.9b00207

33. 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.

32. 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

31. 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

30. 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.

29. 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

28. **M. Bernardi** and J. C. Grossman
Photovoltaics: Advances in First Principles Modeling - Overview.
Handbook of Materials Modeling: Applications: Current and Emerging Materials **2018**, pages 1-8.
DOI: 10.1007/978-3-319-50257-1_143-1

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 articles 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 feature 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 1300 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 articles 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