Douglas H. Fabini

Massachusetts Institute of Technology Department of Chemistry, Room 6-418 32 Vassar St. Cambridge, MA 02139 dougfabini.github.io fabini@mit.edu

Education

Ph.D. Materials Science University of California, Santa Barbara Advisor: Prof. Ram Seshadri	2014 – 2018
B.S. Mechanical Engineering University of California, Berkeley Highest Honors	2007 – 2011
Fellowships, Scholarships & Recognition	
Alexander von Humboldt Postdoctoral Research Fellowship	2019 – 2021
National Science Foundation Graduate Research Fellowship	2016 - 2018
Excellence in Education Outreach Award, UCSB Materials Research Laboratory	2018
Best student speaker award, UCSB Chemical Sciences Seminar Series	2016
Ed Kramer Award for Best Poster, UCSB Materials Research Outreach Program Symposium	2016
UCSB Materials Research Laboratory & Dow Materials Institute Travel Fellowship (4x)	2015 – 2017
Honorable Mention, National Science Foundation Graduate Research Fellowship	2015
Chancellor's Fellowship, UC Santa Barbara	2014 - 2016
EERE Science & Technology Policy Junior Fellowship, U.S. Department of Energy	2012 - 2014
Highest Honors in Mechanical Engineering, UC Berkeley	2011
Regents' & Chancellor's Scholarship, UC Berkeley	2007 - 2011
Cal Alumni Association Leadership Award Scholarship, UC Berkeley	2007 - 2011
Eagle Scout, Boy Scouts of America	2006
Research & Professional Experience	

Jan 2022 - present

Aug 2018 - Dec 2021

Sep 2014 - Aug 2018

May 2014 - July 2014

Jan 2012 - Mar 2014

Nov 2011 - Dec 2011

Jun 2011 – Aug 2011

Jan 2010 - May 2011

Jul 2009 - May 2010

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Massachusetts Institute of Technology (Cambridge, MA)

IBM Research (Nairobi, Kenya)

Makani Power (Alameda, CA)

U.S. Department of Energy (Washington, DC)

Haath Mein Sehat (Berkeley, CA & Hubli, India)

Max Planck Institute for Solid State Research (Stuttgart, Germany)

UC Santa Barbara Materials Research Laboratory (Santa Barbara, CA)

Cal Energy Corps at Indian Institute of Technology (Kharagpur, India)

UC Berkeley Center for Environmental Design Research (Berkeley, CA)

UC Berkeley Manufacturing Institute (Berkeley, CA)

May 2009 - May 2010

UC Berkeley Thermal Hydraulics Laboratory (Berkeley, CA)

May 2008 - May 2009

Publications, submitted or in press

- 30. D. Fabini(†), K. Honasoge, A. Cohen, S. Bette, K. McCall, C. Stoumpos, S. Klenner, M. Zipkat, L. Hoang, J. Nuss, R. Kremer, M. Kanatzidis, O. Yaffe, S. Kaiser, B. Lotsch, Noncollinear electric dipoles in a polar, chiral phase of CsSnBr₃ perovskite, *submitted*. [arXiv:2401.07978] (†) *corresponding author*
- 29. S. Caicedo-Dávila, A. Cohen, S. Motti, M. Isobe, K. McCall, M. Grumet, M. Kovalenko, O. Yaffe, L. Herz, D. Fabini(†), D. Egger(†), Disentangling the effects of structure and lone-pair electrons in the lattice dynamics of halide perovskites, *submitted*. [arXiv:2310.03408] (†) *corresponding authors*

Publications, appeared

- 28. R. Calaminus, S. Harm, A.-K. Hatz, D. Fabini, I. Moudrakovski, B. Lotsch, Enhancing ionic conductivity by in-situ formation of Li₇SiPS₈ / argyrodite hybrid solid electrolytes, *Chem. Mater.* **2022**, *34*, 7666–7677. [doi] [pdf]
- 27. A. Chow, X. Zhong, D. Fabini, M. Zeller, C. Oertel, $(C_5H_6N)Pb_2X_5$ (X = Cl, Br): Hybrid lead halides based on seven-coordinate Pb(II), *Inorg. Chem.* **2022**, *61*, 6530–6538. [doi]
- 26. A. Cohen, T. Brenner, J. Klarbring, R. Sharma, D. Fabini, R. Korobko, P. Nayak, O. Hellman, O. Yaffe, Diverging expressions of anharmonicity in halide perovskites, *Adv. Mater.* **2022**, *34*, 2107932. [doi]

EDITORS' SUGGESTION

- A. Leonhardt, M. Hirschmann, N. Heinsdorf, X. Wu, D. Fabini, A. Schnyder, Symmetry-enforced topological band crossings in orthorhombic crystals: Classification and materials discovery, *Phys. Rev. Mater.* 2021, 5, 124202. [doi] [pdf]
- 24. L. Gao(*), L. Yadgarov(*), R. Sharma, R. Korobko, K. McCall, D. Fabini, C. Stoumpos, M. Kanatzidis, A. Rappe, O. Yaffe, Metal cation s lone-pairs increase octahedral tilting instabilities in halide perovskites, *Mater. Adv.* **2021**, *2*, 4610–4616. [doi] [pdf] (*) equal contribution
- 23. M. Hirschmann, A. Leonhardt, B. Kilic, D. Fabini, A. Schnyder, Symmetry-enforced band crossings in tetragonal materials: Dirac and Weyl degeneracies on points, lines, and planes, *Phys. Rev. Mater.* **2021**, 5, 054202. [doi] [pdf]
- 22. L. Diehl(*), D. Fabini(*), N. Vargas-Barbosa, A. Jiménez-Solano, T. Block, V. Duppel, I. Moudrakovski, K. Küster, R. Pöttgen, B. Lotsch, Interplay between valence band tuning and redox stability in SnTiO₃: Implications for directed design of photocatalysts, *Chem. Mater.* **2021**, *33*, 2824–2836. [doi] [pdf] (*) equal contribution
- 21. J. Blahusch, D. Fabini(†), A. Jiménez-Solano, B. Lotsch(†), Beyond templating: Electronic structure impacts of aromatic cations in organic–inorganic antimony chlorides, *Z. Anorg. Allg. Chem.* **2021**, *647*, 857–866. [doi] [pdf] (†) corresponding authors

INVITED

- 20. D. Fabini(†), R. Seshadri(†), M. Kanatzidis(†), The underappreciated lone pair in halide perovskites underpins their unusual properties, *MRS Bull.* **2020**, *45*, 467–477. [doi] [pdf] (†) *corresponding authors*
- 19. D. Fabini(†), M. Koerner, R. Seshadri(†), Candidate inorganic photovoltaic materials from electronic structure-based optical absorption and charge transport proxies, *Chem. Mater.* **2019**, *31*, 1561–1574. [doi] [data] (†) *corresponding authors*

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- 18. H. Evans, J. Andrews, D. Fabini, M. Preefer, G. Wu, A. Cheetham, F. Wudl, R. Seshadri, The capricious nature of iodine catenation in I₂ excess, perovskite-derived hybrid Pt(IV) compounds, *Chem. Commun.* **2019**, *55*, 588–591. [doi]
- 17. H. Evans, D. Fabini, J. Andrews, M. Koerner, M. Preefer, G. Wu, F. Wudl, A. Cheetham, R. Seshadri, Hydrogen bonding controls the structural evolution in perovskite-related hybrid platinum(IV) iodides, *Inorg. Chem.* **2018**, *57*, 10375–10382. [doi]
- 16. G. Alexander, D. Fabini, R. Seshadri, M. Kanatzidis, AuPb₂I₇: A narrow bandgap Au³⁺ iodide semiconductor, *Inorg. Chem.* **2018**, *57*, 804–810. [doi]
- 15. E. Schueller, G. Laurita, D. Fabini, C. Stoumpos, M. Kanatzidis, R. Seshadri, Crystal structure evolution and notable thermal expansion in hybrid perovskites formamidinium tin iodide and formamidinium lead bromide, *Inorg. Chem.* **2018**, *57*, 695–701. [doi]



- 14. D. Fabini, T. Siaw, C. Stoumpos, G. Laurita, D. Olds, K. Page, J. Hu, M. Kanatzidis, S. Han, R. Seshadri, Universal dynamics of molecular reorientation in hybrid lead iodide perovskites, *J. Am. Chem. Soc.* **2017**, *139*, 16875–16884. [doi]
- 13. G. Laurita, D. Fabini, C. Stoumpos, M. Kanatzidis, R. Seshadri, Chemical tuning of dynamic cation off-centering in the cubic phases of hybrid tin and lead halide perovskites, *Chem. Sci.* **2017**, *8*, 5628–5635. [doi] [pdf]
- 12. E. Liu, C. Gang, M. Zeller, D. Fabini, C. Oertel, Ligand-induced variations in symmetry and structural dimensionality of lead oxide carboxylates, *Cryst. Growth Des.* **2017**, *17*, 1574–1582. [doi]

INVITED

- 11. D. Fabini, J. Labram, A. Lehner, J. Bechtel, H. Evans, A. Van der Ven, F. Wudl, M. Chabinyc, R. Seshadri, Main-group halide semiconductors derived from perovskite: Distinguishing chemical, structural, and electronic aspects, *Inorg. Chem.* **2017**, *56*, 11–25. [doi] (*Forum Article*)
- 10. D. Fabini, C. Stoumpos, G. Laurita, A. Kaltzoglou, A. Kontos, P. Falaras, M. Kanatzidis, R. Seshadri, Reentrant structural and optical properties and large positive thermal expansion in perovskite formamidinium lead iodide, *Angew. Chem. Int. Ed.* **2016**, *55*, 15392–15396. [doi]
- 9. D. Fabini(*), G. Laurita(*), J. Bechtel, C. Stoumpos, H. Evans, A. Kontos, Y. Raptis, P. Falaras, A. Van der Ven, M. Kanatzidis, R. Seshadri, Dynamic stereochemical activity of the Sn²⁺ lone pair in perovskite CsSnBr₃, *J. Am. Chem. Soc.* **2016**, *138*, 11820–11832. [doi] (*) equal contribution
- 8. H. Evans, A. Lehner, J. Labram, D. Fabini, O. Barreda, S. Smock, G. Wu, M. Chabinyc, R. Seshadri, F. Wudl, (TTF)Pb₂I₅: A radical cation-stabilized hybrid lead iodide with synergistic optoelectronic signatures, *Chem. Mater.* **2016**, *28*, 3607–3611. [doi]
- 7. D. Fabini, T. Hogan, H. Evans, C. Stoumpos, M. Kanatzidis, and R. Seshadri, Dielectric and thermodynamic signatures of low temperature glassy dynamics in the hybrid perovskites CH₃NH₃PbI₃ and HC(NH₂)₂PbI₃, *J. Phys. Chem. Lett.* **2016**, *7*, 376–381. [doi]
- 6. A. Lehner, D. Fabini, H. Evans, C.-A. Hébert, S. Smock, J. Hu, H. Wang, J. Zwanziger, M. Chabinyc, and R. Seshadri, Crystal and electronic structures of complex bismuth iodides $A_3Bi_2I_9$ (A = K, Rb, Cs) related to perovskite: Aiding the rational design of photovoltaics, *Chem. Mater.* **2015**, *27*, 7137–7148. [doi]
- 5. A. Lehner, H. Wang, D. Fabini, C. Liman, C.-A. Hébert, E. Perry, M. Wang, G. Bazan, M. Chabinyc, and R. Seshadri, Electronic structure and photovoltaic application of BiI₃, *Appl. Phys. Lett.* **2015**, *107*, 131109. [doi]

INVITED

4. D. Fabini(†), Quantifying the potential for lead pollution from halide perovskite photovoltaics, *J. Phys. Chem. Lett.* **2015**, *6*, 3546–3548. [doi] [pdf] (*Viewpoint*) (†) *corresponding author*

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- 3. J. Labram, D. Fabini, E. Perry, A. Lehner, H. Wang, A. Glaudell, G. Wu, H. Evans, D. Buck, R. Cotta, L. Echegoyen, F. Wudl, R. Seshadri, and M. Chabinyc, Temperature-dependent polarization in field-effect transport and photovoltaic measurements of methylammonium lead iodide, *J. Phys. Chem. Lett.* **2015**, *6*, 3565–3571. [doi]
- 2. D. Fabini, D. Baridó, A. Omu, and J. Taneja, Mapping induced residential demand for electricity in Kenya, In *Proceedings of the 5th ACM Symposium on Computing for Development (DEV-5)*, San Jose, CA, USA, December 5–6, 2014, 43–52. [doi] [pdf]
- 1. T. Clasen, D. Fabini, S. Boisson, J. Taneja, J. Song, E. Aichinger, A. Bui, S. Dadashi, W. Schmidt, Z. Burt, and K. Nelson. Making sanitation count: Developing and testing a device for assessing latrine use in low-income settings, *Environ. Sci. Technol.* **2012**, *46*, 3295–3303. [doi] [pdf]

Presentations (invited)

Bates College (Lewiston, ME)

Mar 2023

"Pushing electrons uphill: Chemical reduction of transition metals"

Atomic-Level Characterization of Hybrid Perovskites (nanoGe HPATOM2)

Feb 2022

"From local bonding to long-range symmetry-breaking: Polarity, chirality, and the distribution of free carriers in perovskite CsSnBr₃"

Potsdam University, Institute of Chemistry (Potsdam, Germany)

Jun 2021

"Plastic crystal dynamics and property impacts in hybrid lead iodide perovskites," and

"Electrostatics and lone pair covalency place thermodynamic limits on oxide photocatalysts: Lessons from the new SnTiO₃"

Atomic-Level Characterization of Hybrid Perovskites (nanoGe HPATOM)

Jan 2021

"Dynamic, polar distortions in perovskite halides: Origins and impacts"

University of Liverpool, Materials Innovation Factory (Liverpool, UK)

Feb 2020

"Making robust predictions from imperfect quantum chemical calculations: Materials discovery case studies from photovoltaics and topological semimetals"

University of Oxford, Inorganic Chemistry Laboratory (Oxford, UK)

Feb 2020

"Chemical tuning of structure, disorder, and lattice dynamics in perovskite main-group halides"

Second International Seminar on Low-Energy Structural and Electronic Dynamics in Soft Semiconducting Materials (Weizmann Institute of Science, Rehovot, Israel)

Feb 2019

"The unusual role of main-group heavy atom chemistry in the anharmonicity and defect-tolerance of halide perovskites"

UCSB Materials Research Outreach Program (Santa Barbara, CA)

Jan 2018

"Main-group halide perovskites: Structural & dynamical insights for photovoltaic performance

Presentations (contributed)

North American Solid State Chemistry Conference (virtual)

Jul 2021

"Electrostatics and lone pair covalency place thermodynamic limits on oxide photocatalysts: Lessons from the new $SnTiO_3$ "

Materials Research Society Spring Meeting & Exhibit (Phoenix, AZ)

Apr 2018

"High-throughput materials discovery of new photovoltaic absorbers: Taking inspiration from maingroup halide perovskites"

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American Chemical Society National Meeting & Exposition (San Francisco, CA)

"Structure and dynamics of perovskite formamidinium lead iodide: Phase transitions, reentrant prop-

erties, and persistent molecular motion"

International Workshop on Advanced Materials (Ras al-Khaimah, UAE)

Feb 2017

Apr 2017

"Structure and dynamics of perovskite formamidinium lead iodide: Phase transitions, reentrant properties, and persistent molecular motion"

16th Southern School on Computational Chemistry & Materials Science (Jackson, MS)

Jul 2016

"Main-group halide photovoltaics derived from perovskite: Distinguishing chemical, structural, and electronic aspects"

American Chemical Society National Meeting & Exposition (San Diego, CA)

Mar 2016

"Main-group halide perovskites: Local structure and disorder"

Professional Service

Panel Moderator, Science for Energy Policy, nanoGe Spring Meeting

Mar 2021

Reviewer (~8–12x annually) for several ACS, AIP, RSC, Nature Portfolio, APS, and GDCh journals including Chemistry of Materials, JACS, Chemical Science, Angewandte Chemie, Journal of Physical Chemistry, Nature Communications, Applied Physics Letters, APL Materials, PRX Energy, ACS Nano, Journal of Materials Chemistry

Technical & Professional Development

Search Inside Yourself Leadership Program

Jan 23 - 24, 2023

Participant, MIT

Bruker-AXS / MIT Symposium 2022: Modulated Structures

Feb 26, 2022

Participant, MIT Department of Chemistry

Leopoldina-CAS joint conference, "Science for Future - All Starts with Basic Science"

Sep 8 – 11, 2019

Selected participant, University of the Chinese Academy of Sciences, Beijing, China

Training: Leadership Competences for Scientists

Aug 29 - 30, 2019

Participant, Facilitated by Schiller & Mertens GbR @ MPI FKF

Pair Distribution Function Analysis Workshop

Oct 11 - 12, 2018

Participant, Max Planck Insitute for Solid State Research, Stuttgart, Germany

24th WIEN2k Workshop

Sep 18 – 22, 2017

Participant, Insitute of Materials Chemistry, TU Vienna, Austria

17th National School on Neutron & X-ray Scattering

Jun 13 – 27, 2015

Selected participant, Argonne National Laboratory and Oak Ridge National Laboratory

Leadership

MIT Postdoctoral Association (Cambridge, MA)

Apr 2022 – Jan 2024

Recording Secretary & Executive Committee Member

Graduate Scholars Program (UC Santa Barbara, CA)

Jan 2018 - Jun 2018

Advanced Graduate Student Mentor, providing academic, professional, and social resources for a group of STEM graduate students from non-traditional backgrounds

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Sep 2016 – Aug 2017

Outreach Committee Chair, coordinating quarterly outreach event for visiting undergraduate students, developing partnerships with related student organizations

Graduate Students for Diversity in Science (UC Santa Barbara, CA)

Sep 2015 – Aug 2016

Outreach Scheduling, logistics for quarterly outreach event for visiting undergraduate students

Graduate Students for Diversity in Science (UC Santa Barbara, CA)

Sep 2014 – Aug 2015

Lecture Series Advertising, coordinating publicity for quarterly guest speaker series

Haath Mein Sehat (UC Berkeley, CA & Hubli, India)

May 2010 – Jan 2011

Co-President, coordinating water-, sanitation-, and hygiene-related student group projects in Indian urban informal settlements and rural villages, grant writing, interfacing with advisers and field staff, guiding organizational strategy

Pi Tau Sigma Mechanical Engineering Honor Society (UC Berkeley, CA)

Aug 2009 – Jan 2010

Outreach Coordinator, coordinating student involvement in K-12 education and volunteer activities

UC Berkeley Academic Talent Development Program (Richmond, CA)

Jul 2007 & Jul 2008

Instructional Assistant in a fourth grade hands-on summer science class

Teaching

Materials: Structure and Properties I (Materials 100A, UCSB)

Oct 2017

Guest lecturer, delivering undergraduate lectures on atomic structure and interatomic bonding

Introduction to Inorganic Materials (Materials 218, UCSB)

Jan 2016 - Mar 2016

Grader, grading assignments and exams on graduate-level inorganic solid-state chemistry

Thermodynamic Foundations of Materials (Materials 200A, UCSB)

Sep 2015 – Dec 2015

Teaching Assistant, leading recitation sections on graduate-level statistical mechanics and classical thermodynamics, developing homework solutions, grading assignments and exams

Mentoring of Interns

Griheydi Garcia (Manhattan College), BSc intern	Jun 2023 – Aug 2023
Mirjam Zipkat (Ludwig Maximilian University, Munich), MSc intern	Jun 2020 – Aug 2020
Mitchell Koerner (UC Santa Barbara), BSc intern	Nov 2016 – Jun 2018
Vidur Niranian (Natl Inst. of Tech Karnataka India) BSc intern	May 2015 - Jul 2015

Educational Outreach

MIT Chemistry Outreach @ Excel High School (Boston, MA)

May 18, 2023

Pen pal for Letters to a Pre-Scientist (nationwide)

Sep 2022 – May 2023

Event assistance for Girls' Day at Max Planck Institutes FKF & IS (Stuttgart, Germany)

Mar 28, 2019

Family Ultimate Science Exploration, California Nanosystems Institute (UCSB) Oct 2014 – Apr 2018

Teaching hands-on science activities for students and their families on 21 evenings at Carpinteria Middle School (Carpinteria, CA), Santa Barbara Junior High School, La Colina Junior High School, La Cumbre Middle School (Santa Barbara, CA), and Goleta Valley Junior High School (Goleta, CA)

Materials Research Laboratory (UCSB)

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Solar Car Workshop, UCSB Early Academic Outreach Program	Jun 25, 2018	
• Bio-Inspired Robotics, Franklin Elementary School (Santa Barbara, CA)	Jan 8, 2018	
 Montessori Center School (Goleta, CA) 	May 11, 2017	
 Carpinteria Family School (Carpinteria, CA) 	Jan 31, 2017	
 Kellogg Elementary School (Goleta, CA) 	Oct 13, 2016	
• Brandon Elementary School (Goleta, CA)	Jan 28, 2016	
• Bio-Inspired Materials, La Cumbre Junior High School (Santa Barbara, CA)	Jul 27, 2015	
 Monte Vista Elementary School (Santa Barbara, CA) 	Jan 22, 2015	
• Kellogg Elementary School (Goleta, CA)	Oct 16, 2014	
Presenter at Santa Barbara Junior High School Career Day (Santa Barbara, CA)	Feb 23, 2018	
Nano Days exhibitor at Adams Elementary School (Santa Barbara, CA)	Feb 7, 2018	
Judge for Rio Mesa High School Science Fair (Oxnard, CA)	Feb 2, 2018	
Judge for Santa Barbara County Science Fair (Santa Barbara, CA)	Mar 10, 2017	
Presenter of "Toward ubiquitous solar energy: Materials for low cost conversion of sunlight to electricity"		
Laguna Blanca High School @ UCSB (Santa Barbara, CA)	Feb 9, 2017	
Presenter of "Nanotechnology and emerging photovoltaics"		
The Thacher School (Ojai, CA)	Nov 1, 2016	
Presenter of "Solar energy basics & careers in solar energy"		
E.L. Haynes High School (Washington, DC)	Apr 11, 2013	
Hispanic Engineers & Scientists (UC Berkeley)		
Young Engineers & Scientists Day (Berkeley, CA)	Nov 11, 2009	
Berkeley Engineers & Mentors (UC Berkeley)		
Berkeley High School (Berkeley, CA)	Sep 8, 2009	

Please see dougfabini.github.io for the latest version of this document, including updated publications. Academic and professional references and a list of manuscripts in preparation are available upon request.

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