

Douglas H. Fabini

Massachusetts Institute of Technology
Department of Chemistry, Room 56-579
21 Ames St.
Cambridge, MA 02142
dougfabini.github.io
fabini@mit.edu

Education

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| Ph.D. Materials Science University of California, Santa Barbara Advisor: Prof. Ram Seshadri [thesis] | 2014 – 2018 |
| B.S. Mechanical Engineering University of California, Berkeley Highest Honors | 2007 – 2011 |

Fellowships, Scholarships & Recognition

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|---|-------------|
| 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

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|---|----------------------|
| Massachusetts Institute of Technology (Cambridge, MA) | Jan 2022 – present |
| Max Planck Institute for Solid State Research (Stuttgart, Germany) | Aug 2018 – Dec 2021 |
| UC Santa Barbara Materials Research Laboratory (Santa Barbara, CA) | Sep 2014 – Aug 2018 |
| IBM Research (Nairobi, Kenya) | May 2014 – July 2014 |
| U.S. Department of Energy (Washington, DC) | Jan 2012 – Mar 2014 |
| Makani Power (Alameda, CA) | Nov 2011 – Dec 2011 |
| Cal Energy Corps at Indian Institute of Technology (Kharagpur, India) | Jun 2011 – Aug 2011 |
| Haath Mein Sehat (Berkeley, CA & Hubli, India) | Jan 2010 – May 2011 |
| UC Berkeley Center for Environmental Design Research (Berkeley, CA) | Jul 2009 – May 2010 |

UC Berkeley Manufacturing Institute (Berkeley, CA)

May 2009 – May 2010

UC Berkeley Thermal Hydraulics Laboratory (Berkeley, CA)

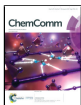
May 2008 – May 2009

Publications

28. R. Calaminus, S. Harm, A.-K. Hatz, D. Fabini, I. Moudrakovski, B. Lotsch, Enhancing ionic conductivity by in-situ formation of Li_7SiPS_8 / argyrodite hybrid solid electrolytes, *submitted*.
27. A. Chow, X. Zhong, D. Fabini, M. Zeller, C. Oertel, $(\text{C}_5\text{H}_6\text{N})\text{Pb}_2\text{X}_5$ ($\text{X} = \text{Cl}, \text{Br}$): 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](#)]
25. 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 SnTiO_3 : 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](#)]
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](#)]
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](#)]
18. H. Evans, J. Andrews, D. Fabini, M. Preefer, G. Wu, A. Cheetham, F. Wudl, R. Seshadri, The capricious nature of iodine catenation in I_2 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, AuPb_2I_7 : A narrow bandgap Au^{3+} 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](#)]

EDITORS'
SUGGESTION

INVITED





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. Chabiniyc, 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 Sn^{2+} lone pair in perovskite CsSnBr_3 , *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. Chabiniyc, R. Seshadri, F. Wudl, $(\text{TTF})\text{Pb}_2\text{I}_5$: 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 $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{HC}(\text{NH}_2)_2\text{PbI}_3$, *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. Chabiniyc, and R. Seshadri, Crystal and electronic structures of complex bismuth iodides $\text{A}_3\text{Bi}_2\text{I}_9$ ($\text{A} = \text{K}, \text{Rb}, \text{Cs}$) 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. Chabiniyc, and R. Seshadri, Electronic structure and photovoltaic application of BiI_3 , *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*)
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. Chabiniyc, 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)

- 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 Feb 2019
in Soft Semiconducting Materials (Weizmann Institute of Science, Rehovot, Israel)
“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 SnTiO₃”
- Materials Research Society Spring Meeting & Exhibit (Phoenix, AZ) Apr 2018
“High-throughput materials discovery of new photovoltaic absorbers: Taking inspiration from main-group halide perovskites”
- American Chemical Society National Meeting & Exposition (San Francisco, CA) Apr 2017
“Structure and dynamics of perovskite formamidinium lead iodide: Phase transitions, reentrant properties, and persistent molecular motion”
- International Workshop on Advanced Materials (Ras al-Khaimah, UAE) Feb 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 for several ACS, AIP, RSC, Nature Portfolio, and GDCh journals including Chemistry of Materials, Journal of Physical Chemistry, Nature Communications, ACS Nano, Applied Physics Letters, APL Materials, Journal of Materials Chemistry, Angewandte Chemie, and Chemical Science

Technical & Professional Development

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 Institute for Solid State Research, Stuttgart, Germany
24th WIEN2k Workshop Sep 18 – 22, 2017
Participant, Institute 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 – present
Recording Secretary
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
Graduate Students for Diversity in Science (UC Santa Barbara, CA) 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

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| Materials: Structure and Properties I (Materials 100A, UCSB) | Oct 2017 |
| <i>Guest lecturer</i> , delivering undergraduate lectures on atomic structure and interatomic bonding | |
| Introduction to Inorganic Materials (Materials 218, UCSB) | Jan 2016 – Mar 2016 |
| <i>Grader</i> , grading assignments and exams on graduate-level inorganic solid-state chemistry | |
| Thermodynamic Foundations of Materials (Materials 200A, UCSB) | Sep 2015 – Dec 2015 |
| <i>Teaching Assistant</i> , leading recitation sections on graduate-level statistical mechanics and classical thermodynamics, developing homework solutions, grading assignments and exams | |

Mentoring of Interns

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| Mirjam Zipkat (Ludwig Maximilian University, Munich), MSc intern | Jun 2020 – Aug 2020 |
| Mitchell Koerner (UC Santa Barbara), BSc intern | Nov 2016 – Jun 2018 |
| Vidur Niranjana (Natl. Inst. of Tech. Karnataka, India), BSc intern | May 2015 – Jul 2015 |

Educational Outreach

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| 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) | |
| • 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.