

Douglas H. Fabini

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Education

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| 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 |

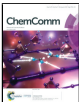
Fellowships, Scholarships & Recognition

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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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|---|----------------------|
| Paul Scherrer Institute (Villigen, Switzerland) | Mar 2025 – present |
| Massachusetts Institute of Technology (Cambridge, MA) | Jan 2022 – Dec 2024 |
| 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 |

Publications

31. E. Riesel, Z. Fang, D. Fabini, A. Altman, Y. Meng, S. Ghose, M. Whitaker, C. Park, D. Popov, A. Rappe, D. Freedman, Planar defect layers template a high-pressure InBi polymorph, *submitted*.
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, *J. Am. Chem. Soc.* **2024**, *146*, 15701. [[doi](#)] [[pdf](#)] (†) *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, *Nat. Commun.* **2024**, *15*, 4184. [[doi](#)] [[pdf](#)] (†) *corresponding authors*
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, (C₅H₆N)Pb₂X₅ (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** 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 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*
-  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. Chabiny, 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. Chabiny, 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. Chabiny, and R. Seshadri, Crystal and electronic structures of complex bismuth iodides A₃Bi₂I₉ (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. Chabiny, 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
3. J. Labram, D. Fabini, E. Perry, A. Lehner, H. Wang, A. Glauddell, G. Wu, H. Evans, D. Buck, R. Cotta, L. Echegoyen, F. Wudl, R. Seshadri, and M. Chabiny, 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)

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| 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 CsSnBr ₃ ” | |
| 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 SnTiO ₃ ” | |
| 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)

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| 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 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

- Reviewer (~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
- Panel Moderator, Science for Energy Policy, nanoGe Spring Meeting Mar 2021

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 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 – 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
- 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

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| Graduate Students for Diversity in Science (UC Santa Barbara, CA) <i>Outreach Scheduling</i> , logistics for quarterly outreach event for visiting undergraduate students | Sep 2015 – Aug 2016 |
| Graduate Students for Diversity in Science (UC Santa Barbara, CA) <i>Lecture Series Advertising</i> , coordinating publicity for quarterly guest speaker series | Sep 2014 – Aug 2015 |
| Haath Mein Sehat (UC Berkeley, CA & Hubli, India) <i>Co-President</i> , 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 | May 2010 – Jan 2011 |
| Pi Tau Sigma Mechanical Engineering Honor Society (UC Berkeley, CA) <i>Outreach Coordinator</i> , coordinating student involvement in K-12 education and volunteer activities | Aug 2009 – Jan 2010 |
| UC Berkeley Academic Talent Development Program (Richmond, CA) <i>Instructional Assistant</i> in a fourth grade hands-on summer science class | Jul 2007 & Jul 2008 |

Teaching

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

Mentoring of Interns

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| 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 Niranjana (Natl. Inst. of Tech. Karnataka, India), BSc intern | May 2015 – Jul 2015 |

Educational Outreach

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| MIT Chemistry Outreach @ Medford High School (Medford, MA) | May 1, 2024 |
| 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) 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) | Oct 2014 – Apr 2018 |
| 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 |

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| • 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.