

Douglas H. Fabini

Paul Scherrer Institut
WHGA/350
Forschungsstrasse 111
5232 Villigen PSI
Switzerland
dougfabini.github.io
dhfabini@gmail.com | douglas.fabini@psi.ch

Education

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

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

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

35. D. Fabini([†]), R. Martyniak, A. Rosa, S. Chariton, E. Riesel, A. Bartlett, E. Mijit, V. Prakapenka, D. Freedman, K₅Ir: Reduced iridium stabilized in a high-pressure semimetal, *submitted*. [[pre-print](#)] ([†]) *corresponding author*
34. J. Ponis, K. Ashen, S. Chakraborty, G. Agbeworvi, M. Smeaton, C. Wang, A. Jessel, D. Fabini, F. Juranyi, D. Quintero-Castro, N. Sheplin, D. Gawryluk, K. Jungjohann, S. Hariyani, X. Qian, S. Banerjee, Alkali-metal interlocking of 2D V₄O₁₀ sheets defines discretized interlayer shear relationships, *submitted*.
33. K. Thanabalasingam, M. Singh, D. Fabini, M. Abeykoon, K. McCall, Discovery of transparent conductor candidate Cs₂CdI₂Cl₂ – Heteroleptic 2D perovskite with 3D electronic character, *submitted*.
32. J. Blahusch, J. Rauh, P. Rovo, I. Moudrakovski, D. Fabini, B. Lotsch, Tuning connectivity in hybrid organic–inorganic antimony halides through reactant concentration effects, *ChemRxiv*. [[pre-print](#)]
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, *J. Am. Chem. Soc.* **2025**, 147, 26496–26505. [[doi](#)]
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, 15701–15717. [[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](#)]
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 SnTiO₃: Implications for directed design of photocatalysts, *Chem. Mater.* **2021**, 33, 2824–2836. [[doi](#)] [[pdf](#)] (*) *equal contribution*

EDITORS' SUGGESTION

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. Schueler, 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. Chabiny, 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. Chabiny, 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) ^(†) corresponding author
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. 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)

Japanese German Symposium on Frontiers in Future Materials Design (MPI FKF, Stuttgart, DE) July 2025	
“Pushing electrons uphill: Reduced transition metals beyond platinide(-II)”	
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)

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
<i>Recording Secretary & Executive Committee Member</i>	
Graduate Scholars Program (UC Santa Barbara, CA)	Jan 2018 – Jun 2018
<i>Advanced Graduate Student Mentor</i> , 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
<i>Outreach Committee Chair</i> , 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
<i>Outreach Scheduling</i> , logistics for quarterly outreach event for visiting undergraduate students	
Graduate Students for Diversity in Science (UC Santa Barbara, CA)	Sep 2014 – Aug 2015
<i>Lecture Series Advertising</i> , coordinating publicity for quarterly guest speaker series	
Haath Mein Sehat (UC Berkeley, CA & Hubli, India)	May 2010 – Jan 2011
<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	
Pi Tau Sigma Mechanical Engineering Honor Society (UC Berkeley, CA)	Aug 2009 – Jan 2010
<i>Outreach Coordinator</i> , coordinating student involvement in K-12 education and volunteer activities	
UC Berkeley Academic Talent Development Program (Richmond, CA)	Jul 2007 & Jul 2008
<i>Instructional Assistant</i> in a fourth grade hands-on summer science class	

Teaching

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

2nd advisor to PhD student Sarbajeet Chakraborty (ETH Zürich)	Jan 2026 – present
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 Niranjan (Natl. Inst. of Tech. Karnataka, India), BSc intern	May 2015 – Jul 2015

Educational Outreach

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)	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.