

# Douglas H. Fabini

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## Education

Ph.D. Materials Science University of California, Santa Barbara Advisor: Prof. Ram Seshadri [ <a href="#">thesis</a> ]	2014 – 2018
B.S. Mechanical Engineering University of California, Berkeley Highest Honors	2007 – 2011

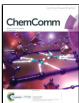

## Fellowships, Scholarships & Recognition

Alexander von Humboldt Postdoctoral Research Fellowship	2019 – present
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

Max Planck Institute for Solid State Research (Stuttgart, Germany)	Aug 2018 – present
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

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 dynamic structural instabilities in halide perovskites, *Mater. Adv.* **2021**, *accepted*. (\*) *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<sub>3</sub>: 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](#)]
- 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](#)]
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<sub>2</sub> 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<sub>2</sub>I<sub>7</sub>: A narrow bandgap Au<sup>3+</sup> 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  $\text{Sn}^{2+}$  lone pair in perovskite  $\text{CsSnBr}_3$ , *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. Chabini, 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. Chabini, 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. Chabini, and R. Seshadri, Electronic structure and photovoltaic application of  $\text{BiI}_3$ , *Appl. Phys. Lett.* **2015**, *107*, 131109. [[doi](#)]
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. Chabini, 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)

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 $\text{SnTiO}_3$ ”	
Atomic-Level Characterization of Hybrid Perovskites (nanoGe HPATOM conference)	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)**

- 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, and GDCh journals including Chemistry of Materials, Journal of Physical Chemistry, ACS Nano, Applied Physics Letters, APL Materials, Journal of Materials Chemistry, and Angewandte Chemie

### **Technical & Professional Development**

- 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
- 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

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 of Interns

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

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

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