

# Dr. Joshua D. Bocarsly

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## EDUCATION

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### UNIVERSITY OF CALIFORNIA, SANTA BARBARA

Sep 2015 – Jun 2020

Santa Barbara, CA

Ph.D. Candidate in Materials (Ph.D. defense: 27 February 2020, degree awarded 10 Jun 2020).

### PRINCETON UNIVERSITY

Sep 2011 – Jun 2015

Princeton NJ, USA

B.A. in Chemistry *Summa Cum Laude*, Certificate in Materials Science and Engineering

## RESEARCH EXPERIENCE

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### POSTDOCTORAL RESEARCH ASSOCIATE

7 Aug 2020 – current

*advisor: Professor Clare Grey, University of Cambridge, Department of Chemistry*

*In situ* studies of magnetic battery materials

*Research objective:* Use magnetic measurements, diffraction, and NMR to understand the electrochemical performance and physical behavior of magnetic battery materials. This research is performed as part of the collaborative, multi-university CATMAT project of the Faraday Institution, seeking to identify and control novel lithium-ion battery materials to enable safe, affordable, well-performing electric vehicles.

### PH.D. RESEARCH

Sep 2015 – Jun 2020

*Co-advisors: Professors Ram Seshadri and Stephen Wilson, UC Santa Barbara, Materials Research Laboratory*

Experimental and computational research in materials chemistry and physics.

*Research objective:* Understand how coupling between magnetism and structure can be used to manipulate magnetic intermetallics, magnetocalorics, and skyrmion-host materials. *Key areas of expertise:* synchrotron and neutron diffraction, magnetic measurements, density functional theory calculations, solid state materials synthesis. Energy materials for applications including magnetocalorics, efficient spintronics, and batteries.

*Roles:* Instrument manager in shared user facility (SQUID and PPMS) and laboratory manager of a synthesis lab.

*Thesis title:* Linking crystal structure and magnetism in intermetallics

### UNDERGRADUATE RESEARCH

1 Feb 2012 – 8 Aug 2015

*Advisor: Professor Robert Cava, Princeton University Chemistry Department*

3.5 years of undergraduate independent research in solid-state chemistry with a focus on the synthesis and characterization (electrical properties, crystal structure, magnetism, and superconductivity) of oxides and oxyfluorides in the tungsten bronze family.

*Thesis title:* Exotic doping schemes in the tungsten bronze family

### OTHER INDEPENDENT RESEARCH:

*June 2012 – Aug 2012:* Summer internship in analytical geochemistry at the Bermuda Institute of Ocean Science (*Advisor:* Dr. Natasha McDonald; *Funder:* Princeton Environmental Institute)

*June 2010 – Aug 2011:* During high school, performed research with Prof. Jeffrey Schwartz (Princeton University) in surface chemistry for biomedical engineering (awarded Intel STS and ISEF finalist for this work)

## SCIENTIFIC COMPUTING

Coursework and independent projects in data processing and analysis, interactive data visualization, machine learning and statistics, and website creation.

Languages: **Scientific Python**, Matlab, R, C, Java, Javascript & HTML

**Publicly available projects:** UCSB Magnet Database ([magnets.mrl.ucsb.edu](https://magnets.mrl.ucsb.edu)) [3], magentro.py code [8]

## AWARDS, PRIZES, AND FELLOWSHIPS

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2019 Marie Curie Individual European Fellowship Reserve List and Seal of Excellence

2016-2019 Six-time awardee of Dow Materials Institute travel fellowships at UC Santa Barbara

- Awarded on the basis of participation in outreach activities, laboratory citizenship, and mentorship.

2019 Member of the U.S. delegation to the Lindau Nobel Laureate meeting (topic: Physics)

- Chosen as one of 67 participants from the U.S. to attend this meeting in Lindau, Germany with 40 Nobel Laureates

2019 Materials Research Laboratory Excellence in Education Outreach Award

- Awarded annually to one or two UC Santa Barbara students in recognition for educational outreach

2019 Edward J. Kramer Prize in Materials

- Inaugural awardee of prize given annually to a UC Santa Barbara student or Post-doc in the field of Materials

2016 NSF Graduate Research Fellowship Awardee

- Competitive US fellowship which completely supports graduate student stipend and tuition for 3 years.

2015-2016 Holbrook Foundation Fellowship, UCSB Institute for Energy Efficiency

- Supplementary fellowship that may be awarded to incoming UC Santa Barbara Ph.D. students

2015 NSF Graduate Research Fellowship Honorable Mention

2015 Henry McCay Prize for Physical Chemistry (Princeton University)

- Awarded to one graduating student annually in the Princeton University Chemistry Department

2015 Election into Sigma Xi, the Scientific Research Society

2011 Intel Science Talent Search Finalist

- Based on independent research carried out in high school. The most prestigious science competition for U.S. high-school students.

2011 Intel International Science & Engineering Fair Finalist

## RESEARCH ARTICLES

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24. Y.M. Oey, D.A. Kitchaev, **J.D. Bocarsly**, E.C. Schueller, J.A. Cooley, R. Seshadri, Magnetocaloric behavior and magnetic ordering in MnPdGa, *submitted*.
23. **J.D. Bocarsly**, M.D. Johannes, S.D. Wilson, R. Seshadri, Magnetostructural coupling from competing magnetic and chemical bonding effects, *submitted*.
22. A.S. Sukhanov, A. Heinemann, L. Kautzsch, **J.D. Bocarsly**, S.D. Wilson, C. Felser, D.S. Inosov, Robust metastable skyrmions with tunable size in the chiral magnet FePtMo<sub>3</sub>N, *accepted to Phys. Rev. B Rapid Communications*.
21. M. B. Preefer, M. Saber, Q. Wei, N.H. Bashian, **J.D. Bocarsly**, W. Zhang, G. Lee, J. Milam-Guerrero, E. S. Howard, R.C. Vincent, B.C. Melot, A. Van der Ven, R. Seshadri, B. Dunn, Multielectron redox and insulator-to-metal transition upon lithium insertion in the fast-charging, Wadsley-Roth phase PNB<sub>9</sub>O<sub>25</sub>, *Chem. Mater.* **32** (2020) 4553-4563. doi:10.1021/acs.chemmater.0c00560
  - Supplementary cover article

20. E.C. Schueller, D.A. Kitchaev, J.L. Zuo, **J.D. Bocarsly**, J.A. Cooley, A. Van der Ven, S.D. Wilson, R. Seshadri, Structural evolution and skyrmionic phase diagram of the lacunar spinel  $\text{GaMo}_4\text{Se}_8$ , *Phys. Rev. Mater.* **4** (2020) 064402. doi: 10.1103/PhysRevMaterials.4.064402
19. Y.M. Oey, **J.D. Bocarsly**, D. Mann, E.E. Levin, M. Shatruk, and R. Seshadri, Structural changes upon magnetic ordering in magnetocaloric  $\text{AlFe}_2\text{B}_2$ , *Appl. Phys. Lett.* **116** (2020) 212403. doi:10.1063/5.0007266
18. A.W. Cook, **J.D. Bocarsly**, R.A. Lewis, A.J. Touchton, S. Morozhnik, T.W. Hayton, An iron ketimide single-molecule magnet  $[\text{Fe}_4(\text{N}=\text{CPh}_2)_6]$  with suppressed through-barrier relaxation, *Chem. Sci.* **11** (2020) 4753. doi: 10.1039/d0sc01578d
17. J.A. Cooley, **J.D. Bocarsly**, E.C. Schueller, E.E. Levin, E.E. Rodriguez, A. Huq, S.H. Lapidus, S.D. Wilson, R. Seshadri, Evolution of non-collinear magnetism in magnetocaloric  $\text{MnPtGa}$ , *Phys. Rev. Mater.* **4** (2020) 044405. doi:10.1103/PhysRevMaterials.4.044405
16. E.E. Levin, **J.D. Bocarsly**, J.H. Grebenkemper, R. Issa, S.D. Wilson, T.M. Pollock, R. Seshadri, Structural coupling and magnetic tuning in  $\text{Mn}_{2-x}\text{Co}_x\text{P}$  magnetocalorics for thermomagnetic power generation, *APL Mater.* **8** (2020) 041106. doi:10.1063/1.5142000
15. L. Kautzsch, **J.D. Bocarsly\***, C. Felser, S.D. Wilson, R. Seshadri, Controlling Dzyaloshinskii-Moriya interactions in the skyrmion host candidates  $\text{FePd}_{1-x}\text{Pt}_x\text{Mo}_3\text{N}$ , *Phys. Rev. Mater.* **4** (2020) 024412. \*corresponding author. doi:10.1103/PhysRevMaterials.4.024412
  - First author was TU Dresden Master's student working under my mentorship.
14. C.A.C. Garcia, **J.D. Bocarsly\***, R. Seshadri, Computational screening of magnetocaloric alloys, *Phys. Rev. Mater.* **4** (2020) 024402. \*corresponding author. doi:10.1103/PhysRevMaterials.4.024402
  - First author was UC Santa Barbara undergraduate under my mentorship
13. A. M. Zieschang, **J.D Bocarsly**, J. Schuch, C. Reichel, B. Kaiser, W. Jaegermann, R. Seshadri, B. Albert, Magnetic and electrocatalytic properties of nanoscale cobalt boride,  $\text{Co}_3\text{B}$ , *Inorg. Chem.* **58** (2019) 16609–16617. doi:10.1021/acs.inorgchem.9b02617
12. M. Preefer, J. Grebenkemper, F. Schroeder, **J.D. Bocarsly**, K. Pilar, J. Cooley, W. Zhang, J. Hu, S. Misra, F. Seeler, K. Schierle-Arndt, R. Seshadri, Rapid and tunable assisted-microwave preparation of glass and glass-ceramic thiophosphate " $\text{Li}_7\text{P}_3\text{S}_{11}$ " Li-ion conductors, *ACS Appl. Mater. Interfaces* **11** (2019) 42280–42287. doi:10.1021/acsami.9b15688
11. E.C. Schueller, J.L. Zuo, **J.D. Bocarsly**, D.A. Kitchaev, S.D. Wilson, and R. Seshadri, Modeling the structural distortion and magnetic ground state of the polar lacunar spinel  $\text{GaV}_4\text{Se}_8$ , *Phys. Rev. B.* **100** (2019) 045131. doi:10.1103/PhysRevB.100.045131
10. **J.D. Bocarsly**, E.E. Levin, S. Humphrey, T. Faske, W. Donner, S.D. Wilson and R. Seshadri, Magnetostructural coupling drives magnetocaloric behavior: The case of  $\text{MnB}$  versus  $\text{FeB}$ , *Chem. Mater.* **31** (2019) 4873–4881 doi:10.1021/acs.chemmater.9b01476
  - Supplementary cover article
9. **J.D. Bocarsly**, C. Heikes, C.M. Brown, R. Seshadri, and S.D. Wilson, Competing magnetic interactions and atomic site preferences in the chiral skyrmion host materials  $\text{Co}_x\text{Zn}_y\text{Mn}_z$  ( $x+y+z=20$ ), *Phys. Rev. Mater.* **3** (2019) 4873–4881, doi:10.1103/PhysRevMaterials.3.014402.
  - Editor's suggestion & highlight in 2019 NCNR Annual Report
8. **J.D. Bocarsly**, R.F. Need, R. Seshadri, and S.D. Wilson, Magnetoentropic signatures of skyrmionic phase behavior in  $\text{FeGe}$ . *Phys. Rev. B. Rapid Communication* **97** (2018) 100404(R). doi:10.1103/PhysRevB.97.100404
  - `magnetrop.py` code released publicly
7. A. Zieschang, **J.D. Bocarsly**, M. Dürrschnabel, H. Kleebe, R. Seshadri, B. Albert, Low-temperature synthesis and magnetostructural transition in antiferromagnetic, refractory nanoparticles: chromium nitride,  $\text{CrN}$ , *Chem. Mater.* **30** (2018) 1610–1616. doi:10.1021/acs.chemmater.7b04815
6. J.H. Grebenkemper, **J.D. Bocarsly**, E.E. Levin, G. Seward, C. Heikes, C. Brown, S. Misra, F. Seeler, K. Schierle-Arndt, S.D. Wilson, R. Seshadri, Rapid microwave preparation and composition tuning of the

high-performance magnetocalorics (Mn,Fe)<sub>2</sub>(P,Si), *ACS Appl. Mater. Interfaces* **10** (2018) 7208– 7213. doi:10.1021/acsami.7b16988

5. E.E. Levin, **J.D. Bocarsly**, K.E. Wyckoff, T.M. Pollock, R. Seshadri, Tuning the magnetocaloric response in half-Heusler/Heusler MnNi<sub>1+x</sub>Sb solid solutions, *Phys. Rev. Mater.* **1** (2017) 075003. doi:0.1103/PhysRevMaterials.1.075003
4. C.M. Hamm, **J.D. Bocarsly**, G. Seward, U.I. Kramm, C.S. Birkel, Non-conventional synthesis and magnetic properties of MAX phases (Cr/Mn)<sub>2</sub>AlC and (Cr/Fe)<sub>2</sub>AlC, *J. Mater. Chem. C* **23** (2017) 5555–5832. doi:10.1039/C7TC00112F
  - Showcased article
3. **J.D. Bocarsly**, E.E. Levin, C.A.C. Garcia, K. Schwennicke, S.D. Wilson, R. Seshadri, A simple computational proxy for screening magnetocaloric compounds, *Chem. Mater.* **29** (2017) 1613–1622. doi:10.1021/acs.chemmater.6b04729 UCSB magnet database created in conjunction with this article
2. A. Zieschang, **J.D. Bocarsly**, M. Dürrschnabel, L. Molina-Luna, H. Kleebe, R. Seshadri, B. Albert, Nanoscale iron nitride, ε-Fe<sub>3</sub>N: Preparation from liquid ammonia and magnetic properties, *Chem. Mater.* **29** (2017) 621–628. doi: 10.1021/acs.chemmater.6b04088
1. **J.D. Bocarsly**, D. Hirai, M.N. Ali, R.J. Cava, Superconducting phase diagram of In<sub>x</sub>WO<sub>3</sub> synthesized by indium deintercalation, *Europhysics Lett.* **103** (2013) 17001. doi:10.1209/0295-5075/103/17001
  - Published at the end of second year as an undergraduate

#### INVITED PRESENTATIONS AND SEMINARS

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4. Magnetocaloric materials for next-generation refrigeration and waste heat recovery. *Invited conference presentation at Materials Research Outreach Program, Santa Barbara, Jan 2019.*
3. Magnetostructural coupling in magnetocalorics: the case of MnB *vs.* FeB. *Invited seminar at TU Darmstadt, Germany, September 2018.*
2. IRG 1: Magnetic intermetallic mesostructures. *Invited presentation at MRSEC summer symposium, Santa Barbara, California, July 2018.*
1. Discovery of new magnetocaloric materials through density functional theory screening, rapid synthesis, and rapid measurement. *Invited Eduard Zintl Colloquium at TU Darmstadt, Germany, September 2016.*

#### SELECTED ORAL AND POSTER CONFERENCE PRESENTATIONS

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8. How magnetism and structure couple in magnetocalorics. *Poster presentation at North American Solid State Chemistry Conference, Golden, Colorado, July 2019.*
7. How magnetism and structure couple in magnetocaloric materials. *Oral presentation at American Chemical Society Spring Meeting, Orlando, Florida, April 2019.*
6. Computational and experimental design of magnetocalorics with large magnetostructural coupling. *Oral presentation at Join MMM–Intermag Conference, Washington D.C., Jan 2019.*
5. Subtle first-order transitions in magnetocalorics. *Oral presentation at Thermag VIII, Darmstadt, Germany, September 2018.*
4. Magnetoentropic signatures of phase transitions in room temperature skyrmion host materials. *Oral presentation at American Physical Society March Meeting, Los Angeles, California, March 2018.*
3. Using a dataset of magnetic material properties to screen for magnetocalorics. *Poster presentation at American Chemical Society Spring Meeting, San Francisco, California, April 2017.*
2. Discovery of new magnetocaloric materials through density functional theory screening, rapid synthesis, and rapid measurement. *Oral presentation at Thermag VII, Torino, Italy, September 2016.*
1. Deposition of Lignin as a Significant Source of Chromophoric Dissolved Organic Matter in the North Atlantic Subtropical Gyre. *Poster presentation at American Geophysical Union Fall Meeting, San Francisco, California, December 2012.*

## MENTORING, TEACHING, OUTREACH, AND SERVICE

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During Ph.D., served as a research mentor for three undergraduate students and one Masters student in both experimental and computational projects. Several publications with undergraduate co-authors, and two publications with mentees as the first author where I am the corresponding author.

Served as teaching assistant for UCSB undergraduate Introduction to Materials Science and Grader for Special Topics in Inorganic Materials.

Outreach activities include organizing hands-on activities and organizations at local schools with primarily underrepresented minority populations, serving as a designated answerer on UCSB ScienceLine, and performing outreach at MOXI, the Wolf Museum of Exploration + Innovation.

Reviewer at *Chemistry of Materials* and *Solid State Sciences*