

Dr. Joshua D. Bocarsly

Postdoctoral Research Associate, University of Cambridge

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26 September 2022

EDUCATION

UNIVERSITY OF CALIFORNIA, SANTA BARBARA

Sep 2015 – Jun 2020

Santa Barbara, CA

Ph.D. in Materials

PRINCETON UNIVERSITY

Sep 2011 – Jun 2015

Princeton NJ, USA

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

RESEARCH EXPERIENCE

POSTDOCTORAL RESEARCH ASSOCIATE

Aug 2020 – current

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

co-advisor: Dr. Siân Dutton, University of Cambridge, Cavendish Laboratory

Roles:

Faraday Institution Postdoctoral Fellow (7 Aug 2020 – current): Develop and use *in situ* and *ex situ* 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.

Co-investigator on BIGMAP-SI project (July 2021 – current): Develop web-based tools for interoperable, open, accessible management of digital battery data. This project is funded by a new 2 year Stakeholder Initiative grant within the European BIG-MAP project, providing partial salary support and supporting research costs.

Head of Cambridge Energy Materials BAG at Diamond Light Source (July 2021 – current): Co-organized successful Block Allocation Group (BAG) proposal at Diamond Light Source beamline I11. This BAG secures routine access to high-resolution synchrotron X-ray diffraction for ~60 Cambridge researchers across four research groups working in the field of energy materials. In this role, I also provide workshops and training to new diffraction users and develop hardware and software for efficient *operando* synchrotron diffractions.

Pembroke College, Cambridge, Postdoctoral Research Associate (September 2021 – current):

PH.D. RESEARCH

Sep 2015 – Jun

2020

advisor: Professor Ram Seshadri, UC Santa Barbara, Materials Research Laboratory

co-advisor: Professor Stephen D. Wilson, UC Santa Barbara, Materials Research Laboratory

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.

Dissertation 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.

Dissertation 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)

MENTORING, TEACHING, AND OUTREACH

Mentorship: At Cambridge, served as formal “day-to-day” supervisor for one undergraduate internship, one year-long masters project, and one interdisciplinary Ph.D. project (ongoing). During Ph.D., I served as a research mentor for three undergraduate students and one Masters student in both experimental and computational projects. These projects have in several publications with undergraduate co-authors, including two publications where the mentees are the first author and I served as corresponding author.

Teaching: Served as Teaching Assistant for the UCSB undergraduate course “Introduction to Materials Science” and as Grader for the post-graduate class “Special Topics in Inorganic Materials”. I additionally guest lectured for each of these classes.

Outreach: Throughout my Ph.D., I participated in and organized hands-on science outreach activities in Santa Barbara schools with primarily underrepresented minority populations in order to introduce students to Materials Science. I also served as a designated answerer on UCSB ScienceLine, providing answers to scientific questions raised by schoolchildren. In recognition of outreach, I was awarded the 2019 Materials Research Laboratory Excellence in Education Outreach Award.

OTHER ACTIVITIES

Peer reviewing: Serve as regular reviewer journals including *Advanced Science*, *Chemistry of Materials*, *Journal of Materials Chemistry C*, *Journal of Alloys and Compounds*, *Solid State Sciences*, and *New Journal of Chemistry*.

Member of organizing committee for 2022 Annual Royal Society Solid State Chemistry Conference (<https://sscgxmas2022.weebly.com/>)

Scientific computing: 9 years experience with scientific programming, automation and data visualizations. Examples of projects available at: magnets.mrl.ucsb.edu [3], magentro.py code [8]. Currently, co-developer of a novel data management system for contextualized, linked data.

AWARDS , PRIZES, AND FELLOWSHIPS

2021 Pembroke College, Cambridge Research Associateship

- Competitive research affiliation awarding college membership and discretionary research funds

2020 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 (High School)
- The most prestigious science competition for U.S. high-school students. Awarded based on independent research carried out in high school.
- 2011 Intel International Science & Engineering Fair Finalist (High School)

RESEARCH ARTICLES

29. L.A.V. Nagle-Cocco, **J.D. Bocarsly**, K. Sada, C. Ritter, E. Suard, N.D. Kelly, C. Liu, C.P. Grey, P. Barpanda, S.E. Dutton, Incommensurate magnetic modulation in K-rich cryptomelane, $K_xMn_8O_{16}$ ($x \approx 1.46$), *submitted*. arxiv:2208.12197
28. C. Szczuka, B. Karasulu, M.F. Groh, F.N. Sayed, T.J. Sherman, **J.D. Bocarsly**, S. Vema, S. Menkin, S. Emge, A.J. Morris, C.P. Grey, Forced disorder in the solid solution Li_3P-Li_2S : A new class of fully reduced solid electrolytes for lithium metal anodes, *J. Am. Chem. Soc.* **144** (2022) 16350–16365. doi: 10.1021/jacs.2c01913
27. J.L. Zuo, D. Kitchaev, E.C. Schueller, **J.D. Bocarsly**, R. Seshadri, A. Van der Ven, S.D. Wilson, Magnetoentropic mapping and computational modeling of cycloids and skyrmions in the lacunar spinels GaV_4S_8 and GaV_4Se_8 , *Phys. Rev. Mater.* **5** (2021) 054410. doi: 10.1103/PhysRevMaterials.5.054410
26. Y.M. Oey, D.A. Kitchaev, **J.D. Bocarsly**, E.C. Schueller, J.A. Cooley, R. Seshadri, Magnetocaloric behavior and magnetic ordering in $MnPdGa$, *Phys. Rev. Mater.* **5** (2021) 014414. doi: 10.1103/PhysRevMaterials.5.014414
25. M.M. Bordelon, **J.D. Bocarsly**, L. Posthuma, A. Banerjee, Q. Zhang, S.D. Wilson, Antiferromagnetism and crystalline electric field excitations in tetragonal $NaCeO_2$, *Phys. Rev. B* **103** (2021) 024430. doi: 10.1103/PhysRevB.102.140409
24. **J.D. Bocarsly**, M.D. Johannes, S.D. Wilson, R. Seshadri, Magnetostructural coupling from competing magnetic and chemical bonding effects, *Phys. Rev. Res. Rapid Commun.* **2** (2020) 042048(R). doi: 10.1103/PhysRevResearch.2.042048
23. W. Cai, **J.D. Bocarsly**, A. Gomez, R.J. Letona Lee, A. Metta-Magaña, R. Seshadri, L. Echegoyen, High blocking temperatures for $DyScS$ endohedral fullerene single-molecule magnets, *Chem. Sci.* **11** (2020) 13129. doi: 10.1039/D0SC05265E
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 $FePtMo_3N$, *Phys. Rev. B Rapid Commun.* **102** (2020) 140409(R). doi:10.1103/PhysRevB.102.140409

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 $\text{PNb}_9\text{O}_{25}$, *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 GaMo_4Se_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 AlFe_2B_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 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 authored by Master's student
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 authored by undergraduate intern
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, Co_3B , *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 "Li₇P₃S₁₁" 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 GaV_4Se_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 MnB versus 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 FeGe . *Phys. Rev. B. Rapid Communication* **97** (2018) 100404(R). doi:10.1103/PhysRevB.97.100404
 - magnetro.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, 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)₂(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_{1+x}Sb solid solutions, *Phys. Rev. Mater.* **1** (2017) 075003. doi:10.1103/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)₂AlC and (Cr/Fe)₂AlC, *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. Schwenicke, 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-Fe₃N: 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_xWO₃ 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

SELECTED ORAL AND POSTER CONFERENCE PRESENTATIONS

10. Magnetic properties controlled by short-range structural and spin order in layered thiophosphates, *Poster presentation at Solid State Chemistry Gordon Research Seminar and Gordon Research Conference, New London, New Hampshire, July 2022.*
9. Short-range structural and magnetic order in layered thiophosphates, *oral presentation at CATMAT consortium meeting, Oxford, June 2022.*
8. Understanding novel cathode materials using magnetic measurements. *Virtual oral presentation at Faraday Institution Annual Conference, online, November 2021.*
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.*
7. Magnetocaloric materials for next-generation refrigeration and waste heat recovery. *Invited presentation at Materials Research Outreach Program, Santa Barbara, Jan 2019.*
5. Subtle first-order transitions in magnetocalorics. *Oral presentation at Thermag VIII, Darmstadt, Germany, September 2018.*
4. Magnetostructural coupling in magnetocalorics: the case of MnB vs. FeB. *Invited seminar at TU Darmstadt, Germany, September 2018.*
5. 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. Discovery of new magnetocaloric materials through density functional theory screening, rapid synthesis, and rapid measurement. *Oral presentation at Thermag VII, Torino, Italy, September 2016.*
2. 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.*
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.*