Joshua D. Bocarsly

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CV updated: 27 January 2019

EDUCATION

UNIVERSITY OF CALIFORNIA, SANTA BARBARA *Sep 2015 - current*
Santa Barbara, CA
Ph.D. Candidate 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

PH.D. RESEARCH *10 Sep 2015 – 3 Sep 2019 (expected)*
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. *Roles:* Instrument manager in shared user facility (SQUID and PPMS), and laboratory manager of a synthesis lab space.

UNDERGRADUATE RESEARCH *1 Feb 2012 – 8 Aug 2015*
Advisor: Professor Robert Cava, Princeton University Chemistry Department

Performed 3.5 years of undergraduate independent research in solid-state chemistry with a focus on the synthesis and characterization of oxides and oxyflourides 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, websites.

Languages: **Scientific Python**, Matlab, R, C, Java, Javascript & HTML
Publicly available projects: UCSB Magnet Database (magnets.mrl.ucsb.edu) [4], magentro.py code [9]

AWARDS, PRIZES, AND FELLOWSHIPS

2016-2019 Six-time awardee of Dow Materials Institute travel fellowships
- 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 to be given annually to a UC Santa Barbara student or Post-doc in the field of Materials

2016 NSF Graduate Research Fellowship Awardee
- Competitive fellowship supporting graduate research in the U.S.

2015-2016 Holbrook Foundation Fellowship, UCSB Institute for Energy Efficiency
- Supplementary fellowship 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 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, APPEARED:

1. 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
2. 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 "$Li_7P_3S_{11}$" Li-ion conductors, *ACS Appl. Mater. Interfaces* **11** (2019) 42280–42287. doi:10.1021/acsami.9b15688
3. 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
4. **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
5. **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 $Co_xZn_yMn_z$ (x+y+z=20), *Phys. Rev. Mater.* 3 (2019) 4873-4881, doi:10.1103/PhysRevMaterials.3.014402.
   - Editor's suggestion & will be highlighted in 2019 NCNR Annual Report
6. **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
8. 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
9. 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:0.1103/PhysRevMaterials.1.075003
10. 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
11. **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
12. A. Zieschang, **J.D. Bocarsly**, M. Dürrschnabel, L. Molina-Luna, H. Kleebe, R. Seshadri, B. Albert, Nanoscale iron nitride, ε-Fe_3N: Preparation from liquid ammonia and magnetic properties, *Chem. Mater.* **29** (2017) 621-628. doi: 10.1021/acs.chemmater.6b04088
13. **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

Undergraduate Thesis:

14. **J.D. Bocarsly,** Exotic doping schemes in the tungsten bronze family, Princeton University, 2015.

RESEARCH ARTICLES, SUBMITTED (MANUSCRIPTS AVAILABLE ON REQUEST)

15. J.A. Cooley, **J.D. Bocarsly**, E.E. Levin, A. Huq, S.H. Lapidus, R. Seshadri, Magnetic behavior, magnetostructural coupling, and the magnetocaloric effect in MnPtGa, *submitted*.
16. C.A.C. Garcia, **J.D. Bocarsly***, and R. Seshadri, Computational screening of magnetocaloric alloys, *in pres at Phys. Rev. Mater.*, *corresponding author. arXiv:1911.12218
    - First author was UC Santa Barbara undergraduate mentored by Bocarsly
17. L. Kautzsch, **J.D. Bocarsly***, C. Felser, S.D. Wilson, R. Seshadri, Controlling Dzyaloshinskii-Moriya interactions in the skyrmion hosts $FePd_{1-x}Pt_xMo_3N$, *in press at Phys. Rev. Mater*, *corresponding author. arXiv:2001.06783
    - First author was TU Dresden Master's student mentored by Bocarsly
18. E.E. Levin, **J.D. Bocarsly**, J.H. Grebenkemper, R. Issa, S.D. Wilson, T.M. Pollock, and R. Seshadri, Structural coupling and magnetic tuning in $Mn_{2-x}Co_xP$ magnetocalorics for thermomagnetic power generation, *submitted*.
    - Invited article

Invited Presentations and Seminars

1. Magnetocaloric materials for next-generation refrigeration and waste heat recovery. Invited conference presentation at Materials Research Outreach Program, Santa Barbara, Jan 2019.
2. Magnetostructural coupling in magnetocalorics: the case of MnB vs. FeB. Invited seminar at TU Darmstadt, Germany, September 2018.
3. IRG 1: Magnetic intermetallic mesostructures. Invited presentation at MRSEC summer symposium, Santa Barbara, California, July 2018.
4. 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

1. How magnetism and structure couple in magnetocalorics. *Poster presentation at North American Solid State Chemistry Conference, Golden, Colorado, July 2019.*
2. How magnetism and structure couple in magnetocaloric materials. *Oral presentation at American Chemical Society Spring Meeting, Orlando, Florida, April 2019.*
3. Computational and experimental design of magnetocalorics with large magnetostructural coupling. *Oral presentation at Join MMM-Intermag Conference, Washington D.C., Jan 2019.*
4. Subtle first-order transitions in magnetocalorics. *Oral presentation at Thermag VIII, 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.*
6. Using a dataset of magnetic material properties to screen for magnetocalorics. *Poster presentation at American Chemical Society Spring Meeting, San Francisco, California, April 2017.*
7. Discovery of new magnetocaloric materials through density functional theory screening, rapid synthesis, and rapid measurement. *Oral presentation at Thermag VII, Torino, Italy, September 2016.*
8. 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, and Outreach

During Ph.D., served as a research mentor for three undergraduate students and one Masters student in both experimental and computational projects. Multiple publications with undergraduate co-authors, and two manuscripts in preparation with mentees as the first 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.

RESEARCH HIGHLIGHTS

[11] **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

My Ph.D. research focuses on how crystal structure and magnetism couple to yield functional properties such as the magnetocaloric effect. In the first paper of the UC Santa Barbara effort in magnetocalorics, I designed a simple DFT-based proxy to quickly screen ferromagnets and identify those most likely to be good magnetocalorics. This project identified candidates that has formed the basis for several other research projects by myself and 4 other students/post-docs at UC Santa Barbara. The data collected and aggregated during this project is available online in interactive format at the UCSB Magnet Database (magnets.mrl.ucsb.edu)

[4] **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).

In this project, we studied MnB, a material identified as a good magnetocaloric by the proxy developed in [9]. By using DFT, magnetic measurements, high-resolution synchrotron diffraction and specialized in-field diffraction, we demonstrated that the remarkable magnetocaloric properties of MnB are driven by coupling between the magnetism and structure. This coupling is achieved due to competition between manganese moment formation and one-dimensional boron-boron bond formation. While [9] identified that magnetostructural coupling is related to the magnetocaloric effect in a generic way, this paper advances our understanding by identifying exactly how magnetostructural coupling can arise, and how it drives a strong magnetocaloric effect. This chemical and physical understanding will allow us to move towards rational design of new magnetocalorics.

[6] **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).

In this project, we created a method for mapping out skyrmionic phase diagrams by using magnetic entropy measurements inspired by those used in the magnetocalorics community. This method allows for the efficient and robust identification of subtle magnetic phase transitions that are otherwise very difficult to identify and properly interpret. The code required to perform this analysis was publically released as `magentro.py`, and is currently in widespread use at UC Santa Barbara (*e.g.* in [16]), as well as at other universities. Data from this project was used as the basis for one of three thrusts in a successful NSF MRSEC IRG proposal.