

Eva H. Smith

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Education

Cornell University, Ithaca, NY

Doctor of Philosophy, Materials Science and Engineering, minor in Chemistry

anticipated May 2017

Master of Science, Materials Science and Engineering, minor in Chemistry

August 2013

National Science Foundation Graduate Research Fellow 2010-2013; GPA: 3.9/4.0

Scripps College, Claremont, CA

Bachelor of Arts, Mathematics; **Bachelor of Arts**, Chemistry

May 2009

James E. Scripps Scholar 2005-2009; GPA: 3.9/4.0

Technical Skills

- Experienced with MATLAB, Mathematica, LaTeX, the Vienna Ab initio Simulation Package (VASP)
- Moderately experienced with Python, Bash, Wannier90, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), molecular beam epitaxy (MBE), wet chemistry methods, vacuum deposition methods
- Familiar with Quantum Espresso, scanning electron microscopy (SEM), nuclear magnetic resonance (NMR) spectroscopy, the Stuttgart Tight Binding-Linear Muffin Tin Orbital (TB-LMTO) program

Selected Research Projects: Interfacing Theory and Experiment

Prediction and growth of novel material Ca_2TiO_4

2013-Present

Dept. of Applied Physics and Dept. of Materials Science and Engineering, Cornell University, Ithaca, NY

- Surveyed literature of similar compounds and evaluated the likelihood for success and reasons for failure of both solid-state and molecular beam epitaxy (MBE) methods to grow Ca_2TiO_4
- Integrated the results from previous growth attempts, reported syntheses of related compounds, and novel first-principles calculations to explain the instability of Ca_2TiO_4 as a bulk phase
- Predicted thin-film conditions under which Ca_2TiO_4 would be stable, grew Ca_2TiO_4 using molecular beam epitaxy (MBE) under predicted conditions, and characterized films using X-ray diffraction (XRD)

Integrating first-principles calculations with Pourbaix diagrams to predict solubility

2013

Dept. of Chemistry and Dept. of Materials Science and Engineering, Cornell University, Ithaca, NY

- Assessed the most accurate methods to calculate enthalpy and entropy of novel materials
- Integrated first-principles data (enthalpy of formation) with existing experimental data (Pourbaix diagrams and standard thermodynamic tables) to predict the stability in water of novel oxide materials

Prediction and growth of intermetallic fuel cell catalysts

2009-2011

Department of Materials Science and Engineering, Cornell University, Ithaca, NY

- Calculated predictors of catalytic activity of intermetallics using first-principles methods
- Grew thin film intermetallic composition spreads using magnetron sputtering
- Measured film composition, chemistry, and phase using X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS); performed high-throughput assessment of catalytic activity across composition spreads

Selected Research Projects: Lone Pair Chemistry

Enhancing dielectric constant in halide perovskite solar cell materials

2014-Present

Department of Applied Physics, Cornell University, Ithaca, NY

- Used first-principles calculations to quantify role of the Pb^{2+} lone pair cation in the dielectric constant, bandgap, and polarization of solar cell material $(\text{CH}_3\text{NH}_3)\text{PbI}_3$
- Developed methods for tuning dielectric constant, bandgap, and polarization via lone pair chemistry

Can the Au^- lone pair be made stereoactive?

2014

Materials Research Laboratory, University of California, Santa Barbara, CA

- Initiated contact with collaborator (Ram Seshadri) and suggested avenue for research
- Evaluated novel auride materials as candidates for ferroelectrics with stereoactive Au^- lone pairs using results of first-principles calculations of bandgap, phonon frequencies, and density of states

Role of lone pair chemistry in phase competition of ferroelectric perovskite CsPbF_3

2011-2014

Department of Applied Physics, Cornell University, Ithaca, NY

- Used a variety of first-principles methods to calculate the structure, chemistry, and energetics of CsPbF_3
- Described the competition or cooperation among different classes of structure-stabilizing phase transitions
- Identified symmetry as a mediator between the chemistry of the Cs^+ and Pb^{2+} cations
- Acquired expertise in calculating predictors and indicators of lone pair stereoactivity

Selected Research Projects: Wet Chemistry and Synthesis

- Kinetics of carbonyl insertion at a κ^3 -[NCN]PtMe complex** 2008-2009
Department of Chemistry, Scripps College, Claremont, CA
- Synthesized precursor organometallic Pt-based compound with wet chemistry, vacuum, and glove-box methods
 - Monitored reaction rates via nuclear magnetic resonance (NMR) spectroscopy
- Pore-filling in solid state dye sensitized solar cells** 2008
Department of Materials Science and Engineering, Stanford University, Stanford, CA
- Developed and tested gravimetric method to measure infiltration of hole conductor into TiO₂ films
 - Cross-checked results with scanning electron microscopy (SEM)
- Synthesis of chiral organic Brønsted acids for catalysis** 2007-2008
Department of Chemistry, Scripps College, Claremont, CA
- Synthesized and purified organic compounds using wet chemistry and column chromatography
 - Characterized products with nuclear magnetic resonance (NMR), gas chromatography/mass spectroscopy (GC-MS), and high-pressure liquid chromatography (HPLC)

Selected Leadership and Team Experiences

- Leadership Committee Member, Expanding Your Horizons Conference**, Ithaca, NY 2010-Present
- Worked with 25 other committee members to host annual science outreach conference for 300 young women
 - Organized schedules of 30 volunteers based on volunteer availability and timeline of conference needs
 - Recorded conference multimedia and collaborated with other chairs to use media in advertisements
 - Recruited panelists from professional network, composed panel questions, and moderated panel discussion to communicate the experience of being a female scientist to a non-scientist audience
 - Selected food and paper goods to provide dinner to 250 people while staying within \$500 budget
- Ragnar Relay Race Team-Member**, multiple locations 2012-2014
- Ran multiple 200-mile 24-30 hour overnight relay races on teams with 5-11 others
 - Mediated conflicts among team members by asking questions to understand each party's perspective and needs, facilitating mutual understanding, presenting potential courses of action, and verifying satisfaction with outcome
 - Shared and helped allocate team responsibilities of reserving vans, finding accommodations, and buying food
 - Applied insights from past races to improve future race experiences
- Vice President, President, and Secretary, Graduate Women in Science**, Alpha Chapter, Ithaca, NY 2010-2013
- Increased membership from 2 to 30 through networking, outreach events, and publicity efforts
 - Oversaw the planning and production of professional development and outreach events, including a fellowship application session, science "cabaret," and afternoon of hands-on science activities for young children
 - Led fellowship application sessions in which 10 volunteers gave guidance and feedback to 40 students
 - Recruited volunteers for fellowship application session, reserved meeting space, and organized advertising efforts
- Meeting Co-Chair, Graduate Women in Science National Conference and Symposium**, Ithaca, NY 2011
- Worked closely with co-chair to make decisions regarding conference scope, content, and speakers; delegation of tasks to subcommittees; planning timeline; and oversight of conference organization
 - Attracted 60 women and men nationally to attend conference occupying 2 full days
 - Monitored adherence to planning timeline and worked with subcommittee chairs to address sources of delays
 - Networked with Cornell resources, other academic institutions, industry, and local government to recruit 25 relevant, diverse speakers to serve on panels, give talks, and lead workshops

Teaching and Mentoring Experience

- Undergraduate student mentor** Summer 2012
Department of Applied Physics, Cornell University, Ithaca, NY
- Taught methods to calculate materials properties, find sources in the literature, and verify findings
 - Communicated appropriate style and content for scientific writing and scientific presentations
 - Guided student through project life cycle: literature search, data collection, project refinement, project completion, and results communication
- Teaching Assistant, Mechanical Properties of Materials** Fall 2010
Department of Materials Science and Engineering, Cornell University, Ithaca, NY
- Prepared and taught discussion section or laboratory section 3 times per week
 - Designed homework assignments and wrote homework answer keys every other week
 - Interacted with students and reviewed material in office hours 4 hours per week
 - Wrote instructions for lab, guided students performing the lab, and wrote lab grading keys
 - Assisted with in-class demonstrations during lecture for 2 hours every week

Publications

Smith, E. H., Benedek, N. A. and Fennie, C. J. "Lone Pair Cations Mediate the Interaction of Octahedral Rotations and Ferroelectricity." Manuscript in Preparation.

Birol, T., Benedek, N. A.,... Smith, E. H.,... "The magnetoelectric effect in transition metal oxides: Insights and the rational design of new materials from first principles." *Current Opinion on Solid State and Materials Science*. **16**, 227-242, 2012.

Tague, M. E., Gregoire, J. M., ... Smith, E. H.,... "High Throughput Thin Film Pt-M Alloys for Fuel Electrooxidation: Low Concentrations of M (M = Sn, Ta, W, Mo, Ru, Fe, In, Pd, Hf, Zn, Zr, Nb, Sc, Ni, Ti, V, Cr, Rh)." *Journal of the Electrochemical Society*. **159**, F880-F887, 2012.

Gregoire, J. M., Tague, M. E., Smith, E. H.,... "Phase Behavior of Pseudobinary Precious Metal-Carbide Systems." *Journal of Physical Chemistry C*. **114**, 21664-21671, 2010.

Gutierrez, E. G., Moorhead, E. J., Smith, E. H., ... "Electron-Withdrawing, Biphenyl-2,2'-diol-Based Compounds for Asymmetric Catalysis." *European Journal of Organic Chemistry*. **2010**, 3027-3031, 2010.

Ding, I.-K., Tetreault, N., ... Smith, E. H., ... "Pore-Filling of Spiro-OMeTAD in Solid-State Dye Sensitized Solar Cells: Quantification, Mechanism, and Consequences for Device Performance." *Advanced Functional Materials*. **19**, 2431-2436, 2009.

Posters and Talks

"How stereoactive lone pairs mediate the interaction between ferroelectricity and octahedral rotations in perovskite CsPbF₃." **Poster**, Solid State Chemistry Gordon Conference, 2014. New London, NH.

"How lone pair cations influence the interplay of octahedral rotations and ferroelectricity in CsPbF₃." **Poster**, Fundamental Physics of Ferroelectrics and Related Materials, 2014. Washington, D.C.

"Why is CsPbF₃ ferroelectric, and why is CsSnF₃ not?" **Poster**, North America Solid State Chemistry Conference, 2013. Corvallis, OR.

"Why isn't CsSnF₃ ferroelectric?" **Poster**, Fundamental Physics of Ferroelectrics, 2013. Ames, IO.

"Why is CsPbF₃ ferroelectric?" **Talk**, American Physical Society March Meeting, 2013. Baltimore, MD.

"Surface Electronic Structure of N-doped Pt-Ni Films." **Poster**, Dynamics at Surfaces Gordon Conference, 2011. Newport, RI.

"High throughput methods for electrocatalyst discovery." **Invited poster**, Department of Energy Energy Frontier Research Center Summit and Forum, 2011. Washington, D.C.

"Unique Capabilities Available at Cornell: Combinatorial Methods." **Invited talk**, Energy Material Center at Cornell Review Board Meeting, 2011. Ithaca, NY.

Mechanistic studies of carbonyl insertion at a κ^3 -[NCN]PtMe complex." **Poster**, American Chemical Society National Meeting, 2009. Salt Lake City, UT."