Michael Kocher

Contact Information

San Francisco, CA — e-mail: michael.kocher@me.com

Education

Ph.D. Material Science and Engineering
Arizona State University, Tempe, AZ 85287 — December 2008
Thesis: *The Electronic Structure of Lithium Transition Metal Oxides*

Bachelor of Science in Physics
Arizona State University, Tempe, AZ 85287 — April 2004

Bachelor of Science in Chemistry
Arizona State University, Tempe, AZ 85287 — April 2004

Programming, Tools and Frameworks

Languages: Python, Scala, Ruby

Extensive experience with PBS, Slurm and SGE for running high-throughput computations on HPC systems. MongoDB and SQL for database driven applications and experienced with object-oriented programming using Python and Ruby. Skilled in several web frameworks, such as Django, Flask, Sinatra for designing web applications. 8 years of experience with Vienna *ab initio* Simulation Package (VASP) and Wien2k to compute properties of materials from first principles. Proficient with Bash for general scripting and system administration. Git for source code version control.

Research Interests

High-throughput computing, workflows, *ab initio* materials science and chemistry, document based data storage (MongoDB), machine learning, message queues, scientific gateways and RESTful interfaces for web driven scientific applications.

Awards

LBNL Spot Prize: "For outstanding and inspiring work on the Materials Project" — January 2012

Top Prize in the LBNL 2010 Mobility Contest: — February 2010
"Mobility Materials Genome: iPhone app to accelerate materials design process"

Professional Experience

Postdoctoral Chemist Researcher — January 2009 – April 2012

Environmental Energy Technology Division
Lawrence Berkeley National Lab, Berkeley, CA
Advisor: Dr. Kristin Persson

- Materials Project (`http://www.materialsproject.org`) lead developer and core database administrator
- Designed a distributed high-throughput workflow engine to perform MPI VASP calculations across several HPC centers
- designed NoSQL database driven scientific applications using Django and MongoDB
- Performed calculation to investigate the role of Al substitution in Li transition metal oxides to understand Li diffusion, cation ordering and stability
- Phonon calculations using *ab initio* quantum molecular dynamic simulations on $LiMnO_2$ and $LiMn_2O_4$ to determine thermal free energies and diffusion properties from first principles
- Performed electronic structure calculations on LiC_x and various Li transition metal oxides to understand the charge compensation mechanism during delithation

Graduate Research Assistant — September 2004 – December 2008

Center for Solid State Science
Arizona State University Tempe
Advisor: Prof. Peter Rez

- Electronic Structure of $LiMn_{1/2}Ni_{1/2}O_2$ and $LiMn_{1/3}Ni_{1/3}Co_{1/3}O_2$
- Electronic Structure calculations on $LiFePO_4$ and $FePO_4$
- Surface interactions of Aspartic and Glutamic Acid on $Ca(C_2O_4)(H_2O)$
- Calculations on 5,7 defects in single wall carbon nanotubes

Undergraduate Research Assistant August 2001 – August 2004

Center for Solid State Science
Arizona State University Tempe, AZ
Advisor: Prof. Andrew Chizmeshya

- Performed calculations of $MgCO_3$ and Mg_2SiO_4 to determine elastic constants and free energies to understand chemical reactions in mineral sequestration of CO_2
- Spin polarized calculation to determine the enthalpy of mixing for $Mg_{1-x}Fe_xCO_3$ solid solution to understand the effect of Fe impurities in serpentine on the sequestration process.
- Phonon calculations using quantum molecular dynamic simulations on $MgCO_3$ and Mg_2SiO_4 to determine thermal free energies from first principles

Undergraduate Research Assistant May 2002 August 2004

Center for Solid State Science
Arizona State University Tempe, AZ
Advisor: Prof. Peter Rez

- Electron Energy Loss Spectroscopy calculations of $SrTiO_3$ and $LaTiO_3$ from *ab initio* methods
- Calculations of surface energies of $Ca(C_2O_4)(H_2O)$ and $Ca(C_2O_4)(H_2O)_2$
- Role of acetylene on Ni (110) and (110) and Ni on graphene sheets for understanding of carbon nanotube formation

Undergraduate Research Assistant August 2000 - May 2001

Department of Chemistry
Arizona State University Tempe, AZ
Advisor: Prof. Tim Steimle

- Assisted in High resolution Spectroscopy experiments
- Maintenance of laboratory apparatus
- Programming of EEPROM Pic devices

Selected Publications

M. Kocher and K. Persson, "Li Mobility and the Electronic Structure of $LiMn_{1/3}Ni_{1/3}Co_{1-x}Al_xO_2$ Determined from First-Principles" *Physical Review B* (submitted)

S. Miao, M. Kocher, P. Rez, B. Fultz, R. Yazami, and C. C. Ahn, "Local electronic structure of olivine phases of Li_xFePO_4", *The Journal of Physical Chemistry A*, vol.111, pp.42427, May (2007).

S . Miao, M. Kocher, P. Rez, B. Fultz, Y. Ozawa, R. Yazami, and C. Ahn, "Local electronic structure of layered $Li_xNi_{0.5}Mn_{0.5}O_2$ and $Li_xNi_{1/3}Mn_{1/3}Co_{1/3}O_2$", *Journal of Physical Chemistry B*, vol. 109, no. 49, pp. 2347323479 (2005).

M.P. Kocher, D.A. Muller and P. Rez,, "The Oxygen K Edge in Strontium Titanate and Lanthanum Titanate", *Microscopy and Microanalysis*, (suppl. 2), 9, 842 (2003).

A. V. G. Chizmeshya, M. J. McKelvy, G. Wolf, M. Kocher, D. Gormley, "Quantum Simulations Studies of Olivine Mineral Carbonation", *Proc. 28th International Technical Conference on Coal Utilization & Fuel Systems* 319-330 (2003).

Conference Presentations and Posters

"Using Python to Accelerate Materials Design", Michael Kocher, Dan Gunter and Shreyas Cholia, PyCon, Santa Clara, CA March (2012)

"Using MongoDB for Materials Discovery" Michael Kocher and Dan Gunter, MongoSV, Santa Clara, CA December (2011)

"The Effect of Al Substitution in Lithium Transition Metal Oxides from First-principles" Michael Kocher, Kristin A. Persson and Quentin M. Ramasse. Materials Research Society Spring Meeting, San Francisco, CA April (2010)

"Does Ni change its charge state in $Li(Mn_{0.5}Ni_{0.5})O_2$ cathode materials?" Peter Rez and Michael Kocher. 208 Electrochemical Society Meeting, Los Angeles, California, October (2005)

"Local Electronic Structure of Layered $Li_xMn_{1/3}Ni_{1/3}Co_{1/3}O_2$" Brent Fultz, Shu Miao, Michael Kocher, Peter Rez, Yasuroni Ozawa, Rachid Yazami, and Channing Ahn. 208 Electrochemical Society Meeting, Los Angeles, California, October (2005)

"CO_2 Mineral Carbonation Processes in Olivine Feedstock: Insights from the Atomic Scale Simulation" Andrew V.G. Chizmeshya, Michael J. McKelvy, Deirdre Gormley, Michael Kocher, Ryan Nunez, Young-Chul Kim and Ray Carpenter, Proc. 29th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, Florida, April (2004)

"Exploration of the Role of Heat Activation in Enhancing Serpentine Carbon Sequestration Reactions" Michael J. McKelvy, Andrew V.G. Chizmeshya, Jason Diefenbacher, George Wolf, Brandon Doss, Deirdre Gormley, Michael Kocher, and Hamdallah Bearat, Proc. 29th International Technical Conference on Coal Utilization and Fuel Systems, Clearwater, Florida, April (2004)

Workshops

Summer School of Computational Material Science — July 2006
Ab Initio Molecular Dynamics Simulation Methods in Chemistry
University of Illinois Urbana-Champaign

International Center for Materials Research Summer School — August 2005
First Principles Calculations for Condensed Matter and Nanoscience
University of California Santa Barbara

References

Available on request.