

# Michael Kocher

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## CONTACT INFORMATION

San Francisco, CA

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<https://github.com/mpkocher>

## 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 and Technologies:** Scala, Python, PostgreSQL, MongoDB, R and Git

Experience with Scala, Akka, and Slick to drive scientific applications using an Agile process. MongoDB and SQL for database driven applications and experienced with object-oriented programming using Scala, Python and Ruby. Extensive experience with PBS, Slurm and SGE for running high-throughput computations on HPC systems. 8+ years of experience with Vienna *ab initio* Simulation Package (VASP) and Wien2k to compute properties of materials from first principles. Knowledgeable Bash for general scripting and system administration and R for data analysis.

## RESEARCH INTERESTS

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

## PROFESSIONAL EXPERIENCE

### **Senior Staff Engineer**

June 2015 – present

Pacific Biosciences, Menlo Park, CA

- Secondary Analysis Infrastructure Tech Lead for the Sequel Release (SMRT Link 3.0) and member of the Architectural Review Board (ARB)
- Lead migration from Python/Java to Scala for maintainability (smrtflow)
- Lead author for PacBio workflow engine (pbsmrtpipe)
- Lead author for PacBio python common core library, pbcommand and the (internal) R companion, pbcommandr

### **Senior Scientist, Staff Engineer**

December 2012 – June 2015

Pacific Biosciences, Menlo Park, CA

- Introduced a streaming Monoid-ish model for computing report metrics in pbreports package to address scalability issues and keep memory usage approximately constant.
- Convinced and implemented core testing framework (pysiv) to enable pipeline testing. This framework was folded back into the pipeline engine (pbsmrtpipe) and is still currently in use.
- Contributed to converting pbpy mono-repo into smaller, more maintainable and testable python packages.
- Pipeline feature development and maintenance of the SMRT Analysis 2.x workflow engine.

### **Postdoctoral Chemist Researcher**

January 2009 – April 2012

Lawrence Berkeley National Lab, Berkeley, CA

Environmental Energy Technology Division. Advisor: Dr. Kristin Persson

- Materials Project (<http://www.materialsproject.org>) lead developer and core database administrator. Designed NoSQL database driven scientific applications using Django and MongoDB
- Designed a distributed high-throughput workflow engine to perform MPI VASP calculations across several HPC centers
- 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<sub>2</sub> and LiMn<sub>2</sub>O<sub>4</sub> to determine thermal free energies and diffusion properties from first principles
- Performed electronic structure calculations on LiC<sub>x</sub> and various Li transition metal oxides to understand the charge compensation mechanism during delithiation

PROFESSIONAL  
EXPERIENCE  
(CONT.)

**Graduate Research Assistant**

September 2004 – December 2008

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

- Electronic Structure of  $\text{LiMn}_{1/2}\text{Ni}_{1/2}\text{O}_2$  and  $\text{LiMn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1/3}\text{O}_2$
- Electronic Structure calculations on  $\text{LiFePO}_4$  and  $\text{FePO}_4$
- Surface interactions of Aspartic and Glutamic Acid on  $\text{Ca}(\text{C}_2\text{O}_4)(\text{H}_2\text{O})$
- 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  $\text{MgCO}_3$  and  $\text{Mg}_2\text{SiO}_4$  to determine elastic constants and free energies to understand chemical reactions in mineral sequestration of  $\text{CO}_2$
- Spin polarized calculation to determine the enthalpy of mixing for  $\text{Mg}_{1-x}\text{Fe}_x\text{CO}_3$  solid solution to understand the effect of Fe impurities in serpentine on the sequestration process.
- Phonon calculations using quantum molecular dynamic simulations on  $\text{MgCO}_3$  and  $\text{Mg}_2\text{SiO}_4$  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  $\text{SrTiO}_3$  and  $\text{LaTiO}_3$  from *ab initio* methods
- Calculations of surface energies of  $\text{Ca}(\text{C}_2\text{O}_4)(\text{H}_2\text{O})$  and  $\text{Ca}(\text{C}_2\text{O}_4)(\text{H}_2\text{O})_2$
- 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

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"

SELECTED  
PUBLICATIONS

M. Kocher and K. Persson, "Li Mobility and the Electronic Structure of  $\text{LiMn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1-x}\text{Al}_x\text{O}_2$  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  $\text{Li}_x\text{FePO}_4$ ", *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  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{0.5}\text{O}_2$  and  $\text{Li}_x\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3}\text{O}_2$ ", *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  $\text{Li}(\text{Mn}_{0.5}\text{Ni}_{0.5})\text{O}_2$  cathode materials?” Peter Rez and Michael Kocher. 208 Electrochemical Society Meeting, Los Angeles, California, October (2005)

“Local Electronic Structure of Layered  $\text{Li}_x\text{Mn}_{1/3}\text{Ni}_{1/3}\text{Co}_{1/3}\text{O}_2$ ” Brent Fultz, Shu Miao, Michael Kocher, Peter Rez, Yasuoni Ozawa, Rachid Yazami, and Channing Ahn. 208 Electrochemical Society Meeting, Los Angeles, California, October (2005)

“CO<sub>2</sub> 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.*