

## KRISTIN ASLAUG PERSSON (Née EINARSDOTTER)

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Assistant Professor, UC Berkeley Department of Materials Science and Engineering,  
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### EMPLOYMENT

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2015 – Assistant Professor, Department of Materials Science and Engineering, UC Berkeley, CA  
2014 – Consulting Faculty Member, Stanford University CA  
2013 – 2015 Staff Scientist, Lawrence Berkeley National Laboratory, CA  
2008 – 2013 Chemist Research Scientist, Lawrence Berkeley National Laboratory, CA  
2005 – Senior Scientist, Computational Modeling Consultants Inc., Wellesley, MA  
2007 – 2008 Research Associate, Department of Materials Science and Engineering, MIT  
2004 – 2007 Postdoctoral Associate, Department of Materials Science and Engineering, MIT  
2001 – 2002 Consultant, Computational Modeling Consultants Inc., Wellesley, MA  
2001 – 2002 Postdoctoral Associate, Department of Materials Science and Engineering, MIT

### EDUCATION

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1996 – 2001 Ph.D in Theoretical Physics (Computational Materials Science), Royal Institute of Technology (KTH), Sweden.  
Thesis: *Thermodynamical and Dynamical Instabilities from Ab Initio Electronic-Structure Calculations*: Advisor: Göran Grimvall.  
1991 – 1996 Master of Science in Engineering Physics, Lund Institute of Technology (LTH), Sweden.  
Thesis: *Neutrino Oscillations and the Solar Neutrino Problem*: Advisor Cecilia Jarlskog.

### TEACHING

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2015 – Materials for Energy Applications, MSE 136  
2012 – Guest Lecturer CS267, UC Berkeley (lectures available online)  
2005 – 2007 Co-Lecturer, MIT 3.20, *Materials at Equilibrium*.  
Overall rating **2005: 5.8/7.0**, **2006: 5.7/7.0** and **2007: 5.8/7.0**  
1996 – 1999 Lecturer, KTH 51305, *Mathematical Methods in Physics*.  
1996 – 1997 Teaching Assistant, KTH: 2 courses: *Thermodynamics* and *Statistical Mechanics*.  
1995 – 1996 Teaching Assistant, LTH: 3 courses: *Statics*, *Dynamics*, and *Vector Analysis*.

### GRANTS, AWARDS AND DISTINCTIONS

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- **h-index: 23**
- **Berkeley Lab Science at the Theater**: ‘A Google for Materials’ (2013).  
[www.youtube.com/watch?v=cG1J6zeU0IM](http://www.youtube.com/watch?v=cG1J6zeU0IM)
- **The LBNL Director’s Award for Exceptional Scientific Achievement** (2013).
- **Director and co-founder** of The Materials Project ([www.materialsproject.org](http://www.materialsproject.org)) - a public materials property and design platform based on high-throughput first-principles calculations.
- **PI** for The Materials Project for Functional Electronic Materials Design – a DOE Modeling and Prediction Center encompassing \$11M over 5 years for FY 2012 – FY 2017.

- **PI** of the Cross-cutting Effort in the JCESR funded by DOE BES for \$25M/5 years.
- **Co-PI** for the SI2-SSI Collaborative Research: A Computational Materials Data and Design Environment encompassing \$2M over 5 years for FY 2012 - 2017.
- **Co-PI and Lead** of the Theory Guiding Synthesis Thrust in the EFRC Center for Next-Generation Materials by Design (**CNGMD**) 2014-2018.
- **Co-PI** of the NSF Center for Materials Sustainable Chemistry (CMSC)
- **Co-PI** of The Batteries for Advanced Transportation Technologies (BATT) Program.
- **Co-PI** of the Joint Center of Artificial Photosynthesis (JCAP).
- **Co-PI** of the Applied Battery Research for Transportation (ABR) Program.
- **LBNL LDRDs** 2010-2011 on ‘Accelerated Materials Design through First-Principles Calculations and Data Mining’.
- **Co-founder** of Pellion Technologies, Inc,
- **Recipient, ARPA-E grant** for developing high-energy density Magnesium ion batteries, 2010.
- **Knut and Alice Wallenberg Scholarship** for Young Promising Female Scientists, 2001.
- **Ph. D Scholarship** (full support), Royal Institute of Technology, Sweden, 1996 - 2001.

## SERVICE and OUTREACH

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- **Associate Editor** of the journal **Chemistry of Materials**.
- **Scientific advisory board** member for the NCCR "MARVEL – Materials’ Revolution: Computational Design and Discovery of Novel Materials, Director Nicola Marzari, EPFL Switzerland
- Member of **The Condensed Matter and Materials Research Committee (CMMRC)** - a standing committee responsible for advising the Board on Physics and Astronomy and the National Research Council. 2013 -
- Member of the **MRS Subcommittee** for New Meetings 2012 – 2015
- MGI Ambassador for the **Metals, Mineral, and Metals Society (TMS)**
- Reviewer of **DOE Early Career Awards**, NSF proposals and computing grants, and **CECAM Workshops**
- Representing the Materials Project and LBNL at the **World Economic Forum, Davos** 2014
- Reviewer of **Nature Materials, Chemistry of Materials, Environmental Energy Science, Journal of Electrochemical Society, Journal of Chemical Physics Letters, Journal of Power Sources, Nanoletters** etc.
- LBNL (Recent) Service and Outreach; Presentations to **UC President Napolitano** 2013, **DOE LDRD Committee** 2014, **Assistant Secretary of Energy** Dave Danielson 2014, **40th Anniversary of EETD** 2013, **Associate Director of Science for Basic Energy Sciences** Harriet Kung 2013, **Nigel Gormly, Head of Direct Investment, New Zealand Superannuation Fund & Jagdeep Bachler, Chief Investment Officer** 2014, **NERSC Anniversary** 2014, **LBNL Advisory Board** 2013, **Science at the Theater** 2013, **Division Directors’ Meeting** 2013, **Advanced Manufacturing Workshop UC Berkeley** 2013, **Director of Naval Research** ONR Julie Christadoulou 2013, **ALS Seminar** 2013, **DOW** 2013-2014, **Volkswagen** 2013-2014, **Applied Materials** 2013, **Intermolecular** 2013.
- Symposium organizer MGI PI Meeting, **MRS Fall Meeting 2014** and **Electrochemical Society Fall Meeting 2013**, **MGI Workshop and Innovation Infrastructure 2012** Washington, **IPAM 2013**, **CECAM workshop 2015**,
- **Dinner with a Scientist** for Oakland Elementary School Children, Oakland Zoo May 2013
- Leader of **MGI Committee**, LBNL

- Tutorial on the Materials Project, **MRS Forum 2012**.

#### INVITED and PLENARY TALKS (Dec 2013 - Dec 2015)

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1. The Materials Project, **IDIES Plenary** Johns-Hopkins Baltimore, October 2015
2. A Materials Genome Approach to Design of Novel Materials and Liquids for Energy Conversion and Storage, **IPF-AVS on Mesoscale Science and Technology**, October 2015 San Jose, CA.
3. Accelerated Materials Design through the Materials Project, **Psi-K** September 2015
4. Insight into Solvation, Dynamics and Stability of Electrolytes for the Design of Novel Multivalent Systems from Coupled Molecular Dynamics and First-Principles Modeling, **Electrochemical Society Meeting**, Phoenix October 2015
5. Accelerated Design through the Materials Project, **UC Davis Colloquium**, June 2015
6. **Materials Challenges for Multivalent Energy Storage**, **American Chemical Society**, Denver, March 2015
7. The Materials Project for Accelerated Materials Design, **American Chemical Society**, Denver, March 2015
8. Solvation Structure of Multi-valent Ions for Multivalent Battery Applications and its Implications for Stability and Charge Transfer, **International Battery Association**, Hawaii, January 2015
9. Design of Novel Multivalent Systems for Energy Storage, Boston, **Fall MRS** Dec 2014
10. The Materials Project for Accelerated Materials Design, **DOW invited visit**, Nov 2014
11. The Materials Project, **ENGE, Jeju, South Korea** Nov 2014
12. The Materials Project for Accelerated Materials Design, **Cornell Invited**, Oct 2014
13. The Materials Project Case Study, **ESNET, Washington** Aug 2014
14. The Materials Genome Initiative, **MMM Plenary**, Berkeley Sept 2014
15. Combining Information Technology with First-Principles Modeling towards Materials Design for Energy Applications, **University of Chicago**, Molecular Engineering Colloquium May 2014
16. Integration between Experiments and Modeling, **NIST MGI Symposium** San Francisco May 2014
17. Building Connections between High-throughput First Principles Modeling and Characterization, **Spring MRS 2014**
18. The Materials Project for Accelerated Materials Design, **LLNL Colloquium** April 2014
19. *Ab Initio* Simulations of Battery Materials, **TMS** February 2014
20. Structural and Chemical Transformations in  $\text{Li}_x\text{MnO}_3$  from First-principles Modeling, **International Battery Association, Brisbane Australia**, March 2014
21. The Materials Project and High-Throughput Accelerated Materials Design, **MRS Boston** Dec 2013

#### PUBLICATIONS

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1. Laura C.H. Gerber, Peter D. Frischmann, Frank Y. Fan, Sean E. Doris, Xiaohui Qu, Angelique Scheuermann, Kristin A. Persson, Yet-Ming Chiang, and Brett A. Helms. *3-Dimensional Growth of  $\text{Li}_2\text{S}$  in Lithium-Sulfur Batteries Promoted by a Redox Mediator*, Nano Letters DOI: 10.1021/acs.nanolett.5b04189 (2015) (accepted)
2. Hong Zhu, Geoffroy Hautier, Umut Aydemir, Zachary M. Gibbs, Guodong Li, Saurabh Bajaj, Jan-Hendrik Pohls, Danny Broberg, Wei Chen, Anubhav Jain, Mary Anne White, Mark Asta, G. Jeffrey Snyder, Kristin Persson, and Gerbrand Ceder. *Computational and experimental investigation of  $\text{TmAgTe}_2$  and XYZ2 compounds, a new group of thermoelectric materials identified by first-principles high-throughput screening*, J. Mater. Chem. C 3(40) (2015)
3. Patrick Huck, Daniel Gunter, Shreyas Cholia, Don Winston, Alpha T. N'Diaye, and Kristin Persson. *User applications driven by the community contribution framework MPContribs in the Materials Project*, Concurrency and Computation: Practice and Experience. cpe.3698 (2015)
4. Peter D. Frischmann, Laura C. H. Gerber, Sean E. Doris, Erica Y. Tsai, Frank Y. Fan, Xiaohui Qu, Anubhav Jain, Kristin A. Persson, Yet-Ming Chiang, and Brett A. Helms. *Supramolecular Perylene Bisimide-Polysulfide Gel Networks as Nanostructured Redox Mediators in Dissolved Polysulfide Lithium-Sulfur Batteries*, Chemistry of Materials, 27 (6765-6770) (2015)

5. Maarten de Jong, Wei Chen, Henry Geerlings, Mark Asta, and Kristin Aslaug Persson. *A database to enable discovery and design of piezoelectric materials*, Scientific Data. 2:150053 | DOI: 10.1038/sdata.2015.53 (2015)
6. Patrick Huck, Anubhav Jain, Daniel Gunter, Don Winston, and Kristin Persson. *A Community Contribution Framework for Sharing Materials Data with Materials Project*, e-Science (e-Science), (2015) IEEE 11th International Conference.
7. Ziqin Rong, Rahul Malik, Pieremanuele Canepa, Gopalakrishnan Sai Gautam, Miao Liu, Anubhav Jain, Kristin Persson, and Gerbrand Ceder. *Materials Design Rules for Multi-Valent Ion Mobility in Intercalation Structures*. Chemistry of Materials (2015)
8. Anubhav Jain, Michael Kocher, Shyue Ping Ong, Miriam Brafman, Geoffroy Hautier, Wei Chen, Guido Petretto, Daniel Gunter<sup>3</sup> and Kristin A. Persson, Bharat Medasani, Gian-Marco Rignanese, Xiaohui Qu, *FireWorks: a dynamic workflow system designed for high-throughput applications*, *Concurrency Computat., Pract. Exper.* (2015) DOI: 10.1002/cpe.3505
9. Maarten de Jong, Wei Chen, Thomas Angsten, Anubhav Jain, Randy Notestine, Anthony Gamst, Marcel Sluiter, Chaitanya Krishna Ande, Sybrand van der Zwaag, Jose J Plata, Cormac Toher, Stefano Curtarolo, Gerbrand Ceder, Kristin A. Persson, and Mark Asta, *Charting the complete elastic properties of inorganic crystalline compounds*, Scientific Data DOI: 10.1038/sdata.2015.9 (2015).
10. H. Ding, B. Medasani, W. Chen, K. A. Persson, M. Haranczyk, and M. Asta. *PyDII: A python framework for computing equilibrium intrinsic point defect concentrations and extrinsic solute site preferences in intermetallic compounds*, Computer Physics Communications , 03 (2015).
11. G. S. Gautam, P. Canepa, R. Malik, M. Liu, K. Persson, and G. Ceder. *First-principles evaluation of multi-valent cation insertion into orthorhombic V2O5*. Chem. Commun. , 51:13619 – 13622 (07) (2015).
12. L. Cheng, C. H. Wu, A. Jarry, W. Chen, Y. Ye, J. Zhu, R. Kostecki, K. Persson, J. Guo, M. Salmeron, G. Chen, and M. Doe. *Interrelationships among grain size, surface composition, air stability and interfacial resistance of Al-substituted Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> solid electrolytes*, ACS Applied Materials Interfaces (2015).
13. Pieremanuele Canepa, Gopalakrishnan Sai Gautam, Rahul Malik, Saivenkataraman Jayaraman, Ziqin Rong, Kevin R. Zavadil, Kristin Persson, and Gerbrand Ceder, *Understanding the Initial Stages of Reversible Mg Deposition and Stripping in Inorganic Nonaqueous Electrolytes*, Chemistry of Materials 27(9) 2015
14. Xiaohui Qu, Anubhav Jain, Nav Nidhi Rajput, Lei Cheng , Yong Zhang, Shyue Ping Ong, Miriam Brafman, Edward Maginn, Larry A. Curtiss, Kristin A. Persson. *The Electrolyte Genome project: A big data approach in battery materials discovery*, Materials Science 103, 56-67 (2015).
15. Wenhao Sun, Sai Jayaraman, Wei Chen, Kristin A. Persson and Gerbrand Ceder, *Nucleation of Metastable Aragonite CaCO<sub>3</sub> in Seawater*, PNAS 1423898112 (2015).
16. Qimin Yan, Guo Li, Paul F. Newhouse, Jie Yu, Kristin A. Persson, John M. Gregoire, and Jeffrey B. Neaton, *Mn<sub>2</sub>V<sub>2</sub>O<sub>7</sub>: an Earth Abundant Light Absorber for Solar Water Splitting*, Adv. Energy Mat. 140184, (2015).
17. Nav Nidhi Rajput, Xiaohui Qu, Niya Sa, Anthony K Burrell, and Kristin Aslaug Persson, *The Coupling between Stability and Ion Pair Formation in Magnesium Electrolytes from First-Principles Quantum Mechanics and Classical Molecular Dynamics*, Journal of the American Chemical Society DOI: 10.1021/jacs.5b01004 (2015).
18. Yuyan Shao, Nav Nidhi Rajput, Jianzhi Hu, Mary Hu, Tianbiao Liu, Zhehao Wei, Meng Gu, Xuchu Deng, Suochang Xu, Kee Sung Han, Jiulin Wang, Zimin Nie, Guosheng Li, Kevin R. Zavadil, Jie Xiao, Chongmin Wang, Wesley A. Henderson, Ji-Guang Zhang, Yong Wang, Karl T. Mueller, Kristin Persson, and Jun Liu, *Nanocomposite polymer electrolyte for rechargeable magnesium batteries*, Nano Energy 12, 750–759 (2015).
19. Lei Cheng, Rajeev S. Assary, Xiaohui Qu, Anubhav Jain, Shyue Ping Ong, Nav Nidhi Rajput, Kristin Persson, and Larry A. Curtiss, *Accelerating Electrolyte Discovery for Energy Storage with High-Throughput Screening*, J. Phys. Chem. Lett, 6, 283–291, (2015).
20. Lei Cheng, Wei Chen, Martin Kunz, Kristin Aslaug Persson, Nobumichi Tamura, Guoying Chen, and Marca Maryse Doeff, *Effect of Surface Microstructure on Electrochemical Performance of Garnet Solid Electrolytes*, ACS Appl. Mater. Interfaces, DOI: 10.1021/am508111r

21. Miao Liu, Ziqin Rong, Rahul Malik, Pieremanuele Canepa, Anubhav Jain, Gerbrand Ceder and Kristin Persson, *Spinel Compounds as Multivalent Battery Cathodes: A Systematic Evaluation Based on ab initio Calculations*, Energy Environ. Sci., 2014, DOI:10.1039/C4EE03389B.
22. Shyue Ping Ong, Shreyas Cholia, Anubhav Jain, Miriam Brafman, Dan Gunter, Gerbrand Ceder, and Kristin A. Persson. *The Materials Application Programming Interface (API): A simple, flexible and efficient API for materials data based on REpresentational State Transfer (REST) principles*. Computational Materials Science 97, 207-2015 (2015).
23. Saul H. Lapidus, Nav Nidhi Rajput, Xiaohui Qu, Karena W. Chapman, Kristin A. Persson and Peter J. Chupas, *Solvation structure and energetics of electrolytes for multivalent energy storage*, Phys. Chem. Chem. Phys., 16, 21941-21945, DOI: 10.1039/C4CP03015J (2014).
24. Keesung S. Han, Nav Nidhi Rajput, X Wei, W Wang, Jianzhi Z. Hu, Kristin A. Persson, Karl T. Mueller, *Diffusional motion of redox centers in carbonate electrolytes*, The Journal of Chemical Physics 141 (10), 104509 (2014).
25. Ivano E. Castelli, Falco Huser, Mohnish Pandey, Hong Li, Kristian S. Thygesen, Brian Seger, Anubhav Jain, Kristin Persson, Gerbrand Ceder, and Karsten W. Jacobsen, *New Light Harvesting Materials Using Accurate and Efficient Bandgap Calculations*, Advanced Energy Materials , DOI: 10.1002/aenm.201400915 (2014).
26. Jie Yu, Qimin Yan, Wei Chen, Anubhav Jain, Jeffrey B. Neaton, and Kristin A. Persson; *First-principles study of electronic structure and photocatalytic properties of MnNiO<sub>3</sub> as an alkaline oxygen-evolution photocatalyst*. Chem. Commun. **51**, 2867-2870, (2015)
27. L. Cheng, E. J. Crumlin, W. Chen, R. Qiao, H. Hou, S. F. Lux, V. Zorba, R. Russo, R. Kostecki, Z. Liu, K. Persson, W. Yang, J. Cabana, T. Richardson, G. Chen and Marca Doeff, *The origin of high electrolyte–electrode interfacial resistances in lithium cells containing garnet type solid electrolytes*, Phys. Chem. Chem. Phys., (2014), DOI: 10.1039/C4CP02921F
28. Kim, Jung-Hyun; Huq, Ashfia; Chi, Miaofang; Pieczonka, Nicholas; Lee, Eunseok; Bridges, Craig; Tessema, Misle; Manthiram, Arumugam; Persson, Kristin; Powell, Bob, *Integrated Nano-Domains of Disordered and Ordered Spinel Phases in LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> for Li-Ion Batteries*, Chemistry of Materials, (2014), DOI: 10.1021/cm501203r
29. Eunseok Lee and Kristin Persson, *Structural and Chemical Evolution of the Layered Li-excess Li<sub>x</sub>MnO<sub>3</sub> as a function of Li content from First-Principles Calculations*, Advanced Energy Materials 1400498, (2014), DOI: 10.1002/aenm.201400498.
30. Qiao, R., Lucas, I. T., Karim, A., Syzdek, J., Liu, X., Chen, W., Persson, K., Kostecki, R., Yang, W. (2014). *Distinct Solid-Electrolyte-Interphases on Sn (100) and (001) Electrodes Studied by Soft X-Ray Spectroscopy*. *Adv. Mater. Interfaces*, 1: 1300115 (2014), DOI:10.1002/admi.201300115.
31. Gerbrand Ceder and Kristin Persson, *How Supercomputers Will Yield a Golden Age of Materials Science*, Cover Story, Scientific American Dec. (2013).
32. Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, Kristin A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Mater. **1**, 011002 (2013)
33. Eunseok Lee and Kristin A. Persson, *First-principles study of the nano-scaling effect on the electrochemical behavior in LiNi<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub>*, Nanotechnology **24** 424007 (2013). doi:10.1088/0957-4484/24/42/424007
34. Eunseok Lee and Kristin Persson, *“Solid-Solution Li Intercalation as a Function of Cation Order/Disorder in the High-Voltage Li<sub>x</sub>Ni<sub>0.5</sub>Mn<sub>1.5</sub>O<sub>4</sub> Spinel”*, Chemistry of Materials 25, 2885-2889 (2013).
35. Nadeem Tahir, Altaf Karim, Kristin Aslaug Persson, Syed Tajammul Hussain, Alejandro Gabriele Cruz Gonzalez, Muhammad Usman, Muhammad Naeem, Ruimin Qiao, Wanli Yang, Yi-De Chuang, Zahid Hussain, *Surface Defects: Possible Source of Room Temperature Ferromagnetism in Co Doped ZnO Nanorods*, J. Phys. Chem. C, (2013), 117 (17), pp 8968–8973
36. Altaf Karim, Sonia Fosse and Kristin A. Persson, *Surface structure and equilibrium particle shape of the LiMn<sub>2</sub>O<sub>4</sub> spinel from first-principles calculations*, Phys Rev. B 87 (7), 075322 (2013) DOI: 10.1103/PhysRevB.87.075322, 2013
37. Yabi Wu, Predrag Lazic, Geoffroy Hautier, Kristin Persson and Gerbrand Ceder, *First principles high throughput screening of oxynitrides for water-splitting photocatalysts*, Energy and

- Environmental Science 6 (1) 157-168, (2013) DOI: 10.1039/c2ee23482c.
38. Eunseok Lee and Kristin A. Persson, *Li Absorption and Intercalation in Single Layer Graphene and Few Layer Graphene by First Principles*, Nano Letters, DOI: 10.1021/nl3019164, (2012).
  39. Dan Gunter, Shreyas Cholia, Anubhav Jain, Michael Kocher, Kristin Persson, Lavanya Ramakrishnan, Shyue Ping Ong, Gerbrand Ceder, *Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project*, 5th Workshop on Many-Task Computing on Grids and Supercomputers (MTAGS) (2012), Conference proceedings.
  40. Shyue Ping Ong, William Davidson Richard, Gerbrand Ceder, Anubhav Jain, Michael Kocher, Shreyas Cholia, Daniel Gunter, Kristin A. Persson, Geoffroy Hautier, and Vincent L. Chevrier, *Python Materials Genomics (pymatgen): A Robust, Open-Source Python Library for Materials Analysis*, Computational Materials Science Volume 68, pg. 314–319 (2013).
  41. Kristin A. Persson, Bryn Waldwick, Predrag Lazic, and Gerbrand Ceder, *Prediction of Solid-Aqueous Equilibria: An Effective Scheme to Combine First-Principles Solid Calculations with Experimental Aqueous States*, Physical Review B Phys. Rev. B 85, 235438 (2012).
  42. Göran Grimvall, Blanka Magyari-Köpe, Vidvuds Ozolins, Kristin A. Persson, *Lattice Instabilities in Metallic Elements*, Reviews of Modern Physics 84, 945–986 (2012).
  43. Eunseok Lee and Kristin A. Persson, *Revealing the Coupled Cation Interactions behind the Electrochemical Profile of  $LixNi_{0.5}Mn_{1.5}O_4$* , Energy Environ. Sci. 5, 6047-6051, (2012).
  44. Anubhav Jain, Geoffroy Hautier, Shyue-Ping Ong, Charles J. Moore, Christopher C. Fischer, Kristin A. Persson, Gerbrand Ceder, *Formation Enthalpies by mixing GGA and GGA+U Calculations*, Physical Review B 84, 045115 (2011).
  45. Anubhav Jain, Geoffroy Hautier, Charles J. Moore, Shyue Ping Ong, Christopher C. Fischer, Tim Mueller, Kristin A. Persson, Gerbrand Ceder, *A High-Throughput Infrastructure for Density Functional Theory Calculations*, Comp. Mat. Sci. 50, 2295–2310 (2011).
  46. Kristin Persson, Yoyo Hinuma, Ying Shirley Meng, Anton van der Ven, and Gerbrand Ceder, *Thermodynamic and Kinetic Properties of the Li-Graphite System from First-Principles Calculations*, Physical Review B 82, 125416, (2010).
  47. Kristin Persson, Vijay A. Sethuraman, Laurence H. Hardwick, Yoyo Hinuma, Ying Shirley Meng, Anton van der Ven, Venkat Srinivasan, Robert Kostecki, and Gerbrand Ceder, *Li Diffusion in Graphite*, J Phys Chem. Lett. 1(8) 1176-1180, (2010).
  48. Lei Tang, Byungchan Han, Kristin Persson, Cody Friesen, Ting He, Karl Sieradzki and Gerbrand Ceder, *Electrochemical Stability of Nanometer-Scale Pt Particles in Acidic Environments*, J. Am. Chem. Soc., 132 (2), 596, (2010).
  49. Robert E. Doe, Kristin A. Persson, Geoffroy Hautier, and Gerbrand Ceder, *First Principles Study of the Li-Bi-F Phase Diagram and Bismuth Fluoride Conversion Reactions with Lithium*, Electrochem. Sol. State Lett. 12 (7), A125, (2009)
  50. Lei Bi, Alexander R. Taussig, Hyun-Suk Kim, Lei Wang, Gerald F. Dionne, D. Bono, Kristin Persson, Gerbrand Ceder and C. A. Ross, *Structural, magnetic and optical properties of  $BiFeO_3$  and  $Bi_2FeMnO_6$  epitaxial thin films: an experimental and first principles study*, Phys. Rev. B. 78 (10), 104106, (2008).
  51. Robert E. Doe, Kristin A. Persson, Y. Shirley Meng, and Gerbrand Ceder, *First Principles Investigation of the Li-Fe-F Phase Diagram and Equilibrium and Non-Equilibrium Conversion Reactions of Fe-fluorides with Li*, Chem. Mat. 20 (16) 5274, (2008).
  52. V. Sivakumar, C. A. Ross, N. Yabuuchi, Y. Shao-Horn, K. Persson, and G. Ceder, *Electrochemical Control of the Magnetic Moment of  $CrO_2$* , J Electrochem. Soc. 155 (8), 83 -88, (2008).
  53. Ashley Predith, Chris Wolverton, Kristin Persson, Tim Mueller, and Gerbrand Ceder, *Ab initio prediction of novel ordered structures in  $ZrO_2 - Y_2O_3$* , Phys. Rev. B 77, 144104 (2008).
  54. Amelia Berta, Kristin Persson, and Dane Morgan, *Ab initio Study of the Composition Dependence of the Pressure-induced Spin Transition in the  $(Mg_{1-x}Fe_x)SiO_3$  system*, Earth Plan Sci Lett 265, 535 (2008).
  55. J. M. Gallardo-Amores, N. Biskup, U. Amador, K. Persson, G. Ceder, E. Moran, and M. E. Arroyo y de Dompablo. *Computational and Experimental Investigation of the Transformation of  $V_2O_5$  under pressure*, Chemistry of Materials (2007) DOI: 10.1021/cm071360p. (2006).
  56. Kristin Persson, Gerbrand Ceder, Amelia Berta and Dane Morgan, *Ab initio Study of the Composition Dependence of the Pressure-induced Spin Transition in the  $(Mg_xFe_{1-x})O$  system*,

- Geophys. Res. Lett., 33, L16306 (2006).
57. Kristin Persson, Dane Morgan and Gerbrand Ceder, *Spin Transitions in the  $(Fe_xMn_{1-x})S_2$  system*, Physical Review B 73, 115201 (2006).
  58. Stefano Curtarolo, Dane Morgan, Kristin Persson, John Rogers, and Gerbrand Ceder, *Predicting Crystal Structures with Data Mining of Quantum Calculations*, Physical Review Letters 91, 135503 (2003).
  59. Mathias Ekman, Kristin Persson, and Göran Grimvall, *Lattice dynamics and thermodynamic properties of the beta-Sn phase in Si*, Physical Review B 62, 14784 (2000).
  60. Kristin Persson, Mathias Ekman, and Vidvuds Ozolins, *Phonon instabilities in bcc Sc, Ti, La and Hf*, Physical Review B 61, 11221 (2000).
  61. Mathias Ekman, Kristin Persson, and Göran Grimvall, *Phase diagram and lattice instability in tungsten-rhenium alloys*, Journal of Nuclear Materials 278, 273 (2000).
  62. Kristin Persson, Mathias Ekman, and Göran Grimvall, *Dynamical and thermodynamical instabilities in the disordered  $Re_xW_{1-x}$  system*, Physical Review B 60, 9999 (1999).
  63. Mathias Ekman, Babak Sadigh, Kristin Einarsdotter, and Peter Blaha, *Ab initio study of the martensitic bcc-hcp transformation in iron*, Physical Review B 58, 5296 (1998).
  64. Kristin Einarsdotter, Babak Sadigh, Göran Grimvall, and Vidvuds Ozolins, *Phonon Instabilities in fcc and bcc Tungsten*, Physical Review Letters 79, 2073 (1997).

## PATENTS

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- *Rechargeable magnesium ion cell components and assembly*. R. Doe, K. Persson and G. Blomgren. US Patent 8361661 filed 2011, issued 2013.
- *Cathode Materials for Rechargeable Magnesium Batteries I*. R.Doe, K. Persson, J. Barker, G. Ceder, US Patent 9077032 filed 2011, Issued 2015
- *Cathode Materials for Rechargeable Magnesium Batteries II*. R.Doe, K. Persson, J. Barker, G. Ceder, US Patent 2011.
- *Layered Materials with Improved Magnesium Intercalation for Rechargeable Magnesium Ion Cells I*, Doe, R. E, Downie, C. M. Fischer C., Lane G. H., Morgan, D., Nevin, J., Ceder, G., Persson, K. A., Eaglesham, D. United States Patent Application 20130260238
- *Layered Materials with Improved Magnesium Intercalation for Rechargeable Magnesium Ion Cells II*, Doe, R. E, Downie, C. M. Fischer C., Lane G. H., Morgan, D., Nevin, J., Ceder, G., Persson, K. A., Eaglesham, D. United States Patent Application 20130260225

## ADVISORY COMMITTEES

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Scientific advisory board member for the NCCR "MARVEL – Materials' Revolution: Computational Design and Discovery of Novel Materials, Director Nicola Marzari, EPFL Switzerland.

## COLLABORATORS (2012-2015)

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