Anubhav Jain

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Summary

I work on designing and understanding **new materials** from **computational approaches**. My major expertise is using a technique called **density functional theory** in a **high-throughput** mode to screen thousands of materials for an application. Some areas I have worked on are **Li ion batteries**, **multivalent batteries**, **thermoelectrics**, **photocatalysts**, **solar PV**, and **Hg gas adsorbers**. I am also a major developer of the **Materials Project**, develop **open-source codebases**, and work closely with **supercomputing centers**. I am also interested in applications of **machine learning** and **data mining** in materials science.

I have a blog, **www.hackingmaterials.com**, highlighting some of my research interests. I also have a Twitter feed, **twitter.com/jainpapers**, that summarizes all of my papers in 140 characters or less.

Education and Training

2011 – 2013	**Postdoctoral Fellow at Lawrence Berkeley National Laboratory** Topic: The Materials Project Advisors: Dr. Kristin Persson & Dr. David H. Bailey
2006 – 2011	**Ph.D. at Massachusetts Institute of Technology** Department of Materials Science & Engineering Advisor: Prof. Gerbrand Ceder
2002 – 2006	**Bachelors of Engineering at Cornell University** Applied Engineering Physics Department Advisors: Prof. Alexander Gaeta and Prof. R.B. Van Dover

Publications

1. **Understanding Thermoelectric Properties from High-Throughput Calculations: Trends, Insights, and Comparisons with Experiment**
   Chen W., Pohls J.-H., Hautier G., Broberg D., Bajaj S., Aydemir U., Gibbs Z.M., Zhu H., Asta M., Snyder G.J., Meredig B., White M.A., Persson K.A., Jain A. / *(submitted)*
2. **YCuTe2: A Member of A New Class of Thermoelectric Materials with CuTe4-Based Layered Structure**
   Aydemir U., Pohls J.-H., Zhu H., Hautier G., Bajaj S., Gibbs Z.M., Chen W., Li G., Ohno S., Broberg D., Kang S.D., Asta M., Ceder G., White M.A., Persson K., Jain A., Snyder G.J. / *(submitted)*
3. **Large scale computational screening and experimental discovery of novel materials for high temperature CO_2 capture**
   Dunstan M., Jain A., Liu W., Ong S.P., Liu T., Lee J., Persson K., Scott S.A., Dennis J.S., Grey C.P./ *(submitted)*
4. **The Energy Scale of Inorganic Crystalline Metastability**

Sun W., Dacek S., Ong S.P., Hautier G., Jain A., Richards W., Persson K.A., Ceder G. / *(submitted)*

5. **New Opportunities for Materials Informatics: Resources and Data Mining Techniques for Uncovering Hidden Relationships**
   Jain A., Hautier G., Ong S.P., Persson K. / *(submitted)* ***invited paper**
6. **Computational Predictions of Energy Materials using Density Functional Theory**
   Jain A., Shin Y., Persson K. / *Nature Reviews Materials (2015)* ***invited paper**
7. **Computational and experimental investigation of TmAgTe2 and XYZ2 compounds, a new group of thermoelectric materials identified by first principles high-throughput screening**
   Zhu H., Hautier G., Aydemir U., Gibbs Z.M., Li G., Bajaj S., Pohls J.-H., Broberg D., Chen W., Jain A., Asta M., Snyder G.J., Persson K., Ceder G. / *J. Mater. Chem C (2015)*
8. **Materials Design Rules for Multi-Valent Ion Mobility in Intercalation Structures**
   Rong Z., Malik R., Canepa P., Gopalakrishnan S.G., Liu M., Jain A., Persson K.A., Ceder G. / *Chemistry of Materials (2015)*
9. **Supramolecular Perylene Bisimide-Polysulfide Gel Networks as Nanostructured Redox Mediators in Dissolved Polysulfide Lithium-Sulfur Batteries**
   Frischmann P.D., Gerber L.C.H., Doris S.E., Tsai E.Y., Fan F.Y., Qu X., Jain A., Persson K.A., Chiang Y-M., Helms B.A. / *Chemistry of Materials (2015)*
10. **FireWorks: a Dynamic Workflow System Designed for High-Throughput Applications**
    Jain A., Ong S.P., Chen W., Medasani B., Qu X., Kocher M., Brafman M., Petretto G., Rignanese G.-M., Hautier G., Gunter D., Persson K.A. / *Concurrency and Computation: Practice and Experience (2015)*
11. **Charting the Complete Elastic Properties of Inorganic Crystalline Compounds**
    de Jong M., Chei W., Angsten T., Jain A., Notestine R., Gamst A., Sluiter M., Ande C., van der Zwaag S., Curtarolo S., Toher C., Plata J.J., Ceder G., Persson K., Asta M. / *Nature Scientific Data (2015)*
12. **The Electrolyte Genome Project: A Big Data Approach in Battery Materials Discovery**
    Qu X., Jain A., Rajput N.N., Cheng L., Zhang Y., Ong S.P., Brafman M., Maginn E., Curtiss L.A., Persson K.A. / *Computational Materials Science (2015)*
13. **First-principles study of electronic structure and photocatalytic properties of MnNiO3 as an alkaline oxygen-evolution photocatalyst**
    Yu J., Yan Q., Chen W., Jain A., Neaton J., Persson K.A. / Chemical Communications (2015)
14. **Relating Voltage and Thermal Safety in Li-ion Battery Cathodes: a High-Throughput Computational Study**
    Jain A., Hautier G., Ong S., Dacek S., Ceder G. / Physical Chemistry Chemical Physics (2015)
15. **Accelerating Electrolyte Discovery for Energy Storage by High Throughput Screening**
    Cheng L., Assary R.S., Qu X., Jain A., Ong S.P., Rajput N.N., Persson K.A., Curtiss L.A. / Journal of Physical Chemistry Letters (2015) ***cover article**
16. **The Materials API: A simple, flexible and efficient application programming interface (API) for materials data based on REpresentational State Transfer (REST) Principles.**
    Ong S., Cholia S., Jain A., Brafman M., Gunter D., Ceder G., Persson K.A. / Comp. Mat. Sci (2015)
17. **Spinel Compounds as Multivalent Battery Cathodes: A Systematic Evaluation Based on *ab initio* Calculations**
    Liu M., Rong Z., Malik R., Canepa P., Jain A., Persson K.A., Ceder G. / Energy & Environmental Science (2014)
18. **New Light Harvesting Materials Using Accurate and Efficient Bandgap Calculations**
    Castelli I.E., Huser F., Pandey M., Li H., Thygesen K.S., Seger B., Jain A., Persson K.A., Ceder G., Jacobsen K.W. / Advanced Energy Materials (2014) ***cover article**
19. **Commentary: The Materials Project: A Materials Genome Approach to Accelerating**

Materials Innovation
Jain A.,** Ong S.,** Hautier G., Chen W., Richards W.D., Dacek S., Cholia S., Gunter D., Skinner D., Ceder G., Persson K.A. / Applied Physics Letters Materials (2013) ***invited paper *one of the highest cited papers in the journal's history *cover article** ***equal contributions*

20. **Performance of Genetic Algorithms in Search for Water Splitting Perovskites**
Jain A., Castelli I. E., Hautier G., Bailey D. H., Jacobsen K. W. / J. Materials Science (2013)

21. **Designing Multi-Electron Lithium-Ion Phosphate Cathodes by Mixing Transition Metals**
Hautier G., Jain A., Mueller T., Moore C., Ong S.P., Ceder G. / Chemistry of Materials (2013)

22. **Improved Capacity Retention for $LiVO_2$ by Cr Substitution**
Ma X., Hautier G., Jain A., Doe R., Ceder G. / J. Electrochemical Society (2012)

23. **Python Materials Genomics (pymatgen): A Robust, Open-Source Python Library for Materials Analysis**
Ong S.P, Richard W.D., Jain A., Hautier G., Kocher M., Cholia S., Gunter D., Chevrier V., Persson K., Ceder G. Computational Materials Science (2012)

24. **From the computer to the laboratory: materials discovery and design using first-principles calculations**
Hautier G., Jain A., Ong S. / Journal of Materials Research (2012) ***invited paper**

25. **Carbonophosphates: a new family of cathode materials for Li ion batteries identified computationally**
Chen, H. Hautier G., Jain A., Moore C., Kang B., Doe R., Wu L., Zhu Y., Tang Y., Ceder G. / Chemistry of Materials (2012)

26. **Accuracy of density functional theory in predicting formation energies of ternary oxides from binary oxides and its implication on phase stability**
Hautier G., Ong S.P., Jain A., Moore C., Ceder G. / Physical Review B (2012)

27. **A Computational Investigation of $Li_9M_3(P_2O_7)_3(PO_4)_2$ (M=V,Mo) as Cathodes for Li Ion Batteries**
Jain A., Hautier G., Moore C., Kang B., Lee J., Chen H., Twu N., Ceder G. / J Electrochem Soc. (2011)

28. **Novel mixed polyanions lithium-ion battery cathode materials predicted by high-throughput ab initio computations**
Hautier G., Jain A., Chen H., Moore C., Ong S.P., Ceder G. / Journal of Materials Chemistry (2011)

29. **Evaluation of Tavorite-Structured Cathode Materials for Lithium-Ion Batteries Using High-Throughput Computing**
Mueller T., Hautier G., Jain A., Ceder G. / Chemistry of Materials (2011)

30. **Voltage, Stability and Diffusion Barrier Differences between Sodium-ion and Lithium-ion Intercalation Materials**
Ong S.P., Chevrier V.L., Hautier G., Jain A., Moore C.J., Kim S., Ma X., Ceder G. / Energy & Env. Sci. (2011)

31. **Phosphates as Lithium-Ion Battery Cathodes: An Evaluation Based on High-Throughput *Ab Initio* Calculations**
Hautier G., Jain A., Ong S.P., Kang B.W., Moore C., Doe R., Ceder G / Chemistry of Materials (2011)

32. **Recharging Lithium Battery Research with Ab Initio Methods**
Ceder G., Hautier G., Jain, A., Ong S.P. / MRS Bulletin (2011) ***invited paper **top 10 downloaded MRS 2011**

33. **Formation Enthalpies by Mixing GGA and GGA+U calculations**
Jain A., Hautier G., Ong S.P., Moore C., Fischer C.C., Persson K., Ceder G. / Phys. Rev B (2011)

34. **A High-Throughput Infrastructure for Density Functional Theory Calculations**
Jain A., Hautier G., Moore C., Ong S.P., Fischer C.C., Persson K., Ceder G. / Comp. Mat. Sci. (2011) ***one of the highest cited papers in the journal's history**

35. **Synthesis and Electrochemical Properties of Monoclinic $LiMnBO_3$ as a Li Intercalation Material**
    Kim J.C., Moore C.J., Kang B., Hautier G., Jain A., Ceder G. / Journal of the Electrochemical Society (2011)
36. **Data-mined Ionic Substitution for New Compound Discovery**
    Hautier G., Fischer C.C., Erlacher V., Jain A., Ceder G. / Inorganic Chemistry (2011)
37. **Finding Nature's Missing Ternary Oxide Compounds Using Machine Learning and Density Functional Theory**
    Hautier G., Fischer C.C., Jain A., Mueller T., Ceder G. / Chemistry of Materials (2010)
38. **Thermal Stabilities of Delithiated Olivine MPO_4 (M=Fe,Mn) Cathodes Investigated using First Principles Calculations**
    Ong S.P., Jain A., Hautier G., Kang B., Ceder G. / Electrochemistry Communications (2010)
39. **Ab Initio Screening of Metal Sorbents for Elemental Mercury Capture in Syngas Streams**
    Jain A., Seyed-Reihani S.A., Fischer C.C., Couling D.J., Ceder G., Green W.H. / Chem. Eng. Sci. (2010)
40. **Are you Centered? An Automatic Crystal-Centering Method for High-Throughput Macromolecular Crystallography**
    Jain A., Stojanoff V. / Journal of Synchrotron Radiation (2007)
41. **A Modular Approach to Beam Line Automation: the NIGMS Facility at the NSLS**
    Allaire M., Berntson A., Jain A., Jakoncic J., Kao C.C., Siddons D.R., So I., Venkatagiriyappa V., Yin Z., Stojanoff V. / Synchrotron Radiation News (2005)

Conference Proceedings

1. **Computational methods for evaluating potential sorbent-based synthesis gas cleanup technologies**
   Couling D., Kshitij P., Jain A., Seyed-Reihani S.A., Das U., Ceder G., Green W.H. / Proceedings of International Pittsburgh Coal Conference (2009) 65 (18), 5295-5295
2. **Community Accessible Datastore of High-Throughput Calculations: Experiences from the Materials Project**
   Gunter D., Cholia S., Jain A., Kocher M., Pesson K., Ramakrishnan L., Ong S., Ceder G. / Fifth Workshop on Many-Task Computing on Grids and Supercomputers, Supercomputing (2012)
3. **A community contribution framework for sharing materials data with Materials Project**

   Huck, P, Jain A., Gunter D., Winston D., Persson K. / IEEE 11th International Conference on eScience (2015)

Patents

1. **Tavorite Structured Cathode Materials for Li-Ion Batteries**
   Mueller T., Hautier G., Ceder G., Jain A.
   (utility patent filed August 2012)
2. **Mixed Phosphate-Diphosphate Electrode Materials and Methods of Manufacturing Same**
   Ceder G., Jain A., Hautier G., Daniel R., Kim J.C., Kang B.
   US Patent 9159991, International Patent WO 2012/024001
3. **Carbonophosphate and Related Compounds**
   Ceder G., Chen H., Hauter G., Kang B., Jain A., Doe R.
   (provisional patent filed February 2010, utility patent filed Feb 2011/issued in 2015)
4. **Design of Multi-Electron Li-ion Phosphate Cathodes by Mixing Transition Metals**

Hautier G., Jain A., Mueller T., Ceder G.
(provisional patent filed January 2013, PCT filed Jan 2014)

10 Selected Presentations

1. **New Energy Storage and Energy Generation Materials from First-Principles Calculations**
   DREAMS workshop, May 2015, *Halifax, Nova Scotia, CA (invited talk)*
2. **The Materials Project: An Electronic Structure Database and its Application to Materials Informatics**
   Materials Research Society, December 2014, *Boston MA (invited talk)*
3. **The Materials Project: An Electronic Structure Database for Community-Based Materials Design**
   ICAMM, July 2014, *Nantes France (invited talk)*
4. **The Materials Project: Computing and Sharing a Searchable Database of Materials Properties Using the FireWorks Job Management System**
   Joint Facilities User Forum on Data-Intensive Computing, June 2014, *Oakland CA (invited talk)*
5. **DFT and Materials Informatics: Finding the "needle in the haystack"**
   CAMD Summer School, August 2012, *Lyngby Denmark (invited talk)*
6. **Is it Possible to Design Safe, High-Voltage Cathodes? An Investigation with High-Throughput Computing**
   Electrochemical Society, May 2012, *Seattle WA*
7. **Investigation of $Li_9V_3(P_2O_7)_3(PO_4)_2$ as a Li Intercalation Cathode with DFT Computations**
   Materials Research Society, April 2012, *San Francisco CA*
8. **The Materials Genome Project: Using High-Throughput Computing to Design New Materials for Clean Energy**
   CECAM, May 2011, *Lausanne Switzerland (invited talk)*
9. **High-Throughput Materials Design: DFT Calculations on All Reported Crystal Structures And Beyond**
   CECAM, April 2010, *Lausanne Switzerland (invited talk)*
10. **Screening of Sorbents for Mercury Capture Using Ab Initio Computations**
    American Institute for Chemical Engineers, April 2009, *Tampa FL*

Major awards

- DOE Early Career Award (2015)
- NERSC Achievement Award: Innovative Use of High-Performance Computing
- Luis W. Alvarez Postdoctoral Fellowship
- DOE Computational Science Graduate Fellowship
- John McMullen Scholarship

Professional Activities

- develop and maintain open-source software for running high-throughput calculations at supercomputing centers (FireWorks)
- contribute to several open-source software packages, including pymatgen and MPWorks
- Vice President of NERSC User Group Executive Committee (supercomputing center)
- leader of committee to develop solutions to more efficiently structure queueing policies

at the NERSC supercomputing center

- referee for multiple journals (Physical Review B, Journal of the Electrochemical Society, Anaalen der Physik, and others) and part of several review panels
- member of judging panel, first materials "hackathon" at Materials Research Society Fall 2014
- maintain a blog on computational materials science (www.hackingmaterials.com)
- maintain a Twitter feed summarizing all my papers (twitter.com/jainpapers)

Personal interests

My hobbies and interests include photography, electronic music composition, and doodles that often end up on my presentation slides; more information is at my personal web site (http://www.anubhavjain.net).