Anubhav Jain

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Energy Technologies Area
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Summary

I work on designing and understanding new materials from computational and machine learning approaches. My major areas of expertise are (i) using density functional theory in a high-throughput mode to screen thousands of materials for an application and (ii) applying various types of machine learning (natural language processing, computer vision, etc.) to materials science problems. Some application areas I have worked on are Li ion batteries, multivalent batteries, thermoelectrics, photocatalysts, CO2 capture materials, solar PV, Hg gas adsorbers, and removing contaminants from water. I am the associate director of The Materials Project and on the leadership team for for the DOE DuraMat consortium.

Education and Training

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

Refereed Archival Journal Articles

1. **Automated Defect Identification in Electroluminescence Images of Solar Modules**
   Chen, X.; Karin, T.; Jain, A. Solar Energy 2022, 242, 20–29.
   https://doi.org/10.1016/j.solener.2022.06.031.
2. **How to analyse a density of states**
   Toriyama, M. Y.; Ganose, A. M.; Dylla, M.; Anand, S.; Park, J.; Brod, M. K.; Munro, J. M.; Persson, K. A.; Jain, A.; Snyder, G. J. Materials Today Electronics 2022, 1, 100002.
   https://doi.org/10.1016/j.mtelec.2022.100002.
3. **Text-Mined Dataset of Gold Nanoparticle Synthesis Procedures, Morphologies, and Size Entities**

Cruse, K.; Trewartha, A.; Lee, S.; Wang, Z.; Huo, H.; He, T.; Kononova, O.; Jain, A.; Ceder, G. Sci Data 2022, 9 (1), 234. https://doi.org/10.1038/s41597-022-01321-6.

4. **Photovoltaic Module Antireflection Coating Degradation Survey Using Color Microscopy and Spectral Reflectance**
   Karin, T.; Reed, M.; Rand, J.; Flottemesch, R.; Jain, A. Progress in Photovoltaics 2022, pip.3575. https://doi.org/10.1002/pip.3575.
5. **Recent Advances and Applications of Deep Learning Methods in Materials Science**
   Choudhary, K.; DeCost, B.; Chen, C.; Jain, A.; Tavazza, F.; Cohn, R.; Park, C. W.; Choudhary, A.; Agrawal, A.; Billinge, S. J. L.; Holm, E.; Ong, S. P.; Wolverton, C. npj Comput Mater 2022, 8 (1), 59. https://doi.org/10.1038/s41524-022-00734-6.
6. **Quantifying the Advantage of Domain-Specific Pre-Training on Named Entity Recognition Tasks in Materials Science**
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7. **A Framework for Quantifying Uncertainty in DFT Energy Corrections**
   Wang, A.; Kingsbury, R.; McDermott, M.; Horton, M.; Jain, A.; Ong, S. P.; Dwaraknath, S.; Persson, K. A. Sci Rep 2021, 11 (1), 15496. https://doi.org/10.1038/s41598-021-94550-5.
8. **Thermal Fluids with High Specific Heat Capacity through Reversible Diels-Alder Reactions**
   Lilley, D.; Yu, P.; Ma, J.; Jain, A.; Prasher, R. iScience 2022, 25 (1), 103540. https://doi.org/10.1016/j.isci.2021.103540.
9. **When Band Convergence Is Not Beneficial for Thermoelectrics**
   Park, J.; Dylla, M.; Xia, Y.; Wood, M.; Snyder, G. J.; Jain, A. Nat Commun 2021, 12 (1), 3425. https://doi.org/10.1038/s41467-021-23839-w.
10. **Best Practices in Machine Learning for Chemistry**
    Artrith, N.; Butler, K. T.; Coudert, F.-X.; Han, S.; Isayev, O.; Jain, A.; Walsh, A. Nat. Chem. 2021, 13 (6), 505–508. https://doi.org/10.1038/s41557-021-00716-z.
11. **Efficient Calculation of Carrier Scattering Rates from First Principles**
    Ganose, A. M.; Park, J.; Faghaninia, A.; Woods-Robinson, R.; Persson, K. A.; Jain, A. Nat Commun 2021, 12 (1), 2222. https://doi.org/10.1038/s41467-021-22440-5.
12. **Optimal Band Structure for Thermoelectrics with Realistic Scattering and Bands**
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13. **Compromise between Band Structure and Phonon Scattering in Efficient N-Mg3Sb2-Bi Thermoelectrics**
    Shi, X.; Zhang, X.; Ganose, A.; Park, J.; Sun, C.; Chen, Z.; Lin, S.; Li, W.; Jain, A.; Pei, Y. Materials Today Physics 2021, 18, 100362. https://doi.org/10.1016/j.mtphys.2021.100362.
14. **Phase-Transition-Enhanced Thermoelectric Transport in Rickardite Mineral Cu 3– x Te 2**
    Yahyaoglu, M.; Ozen, M.; Prots, Y.; El Hamouli, O.; Tshitoyan, V.; Ji, H.; Burkhardt, U.; Lenoir, B.; Snyder, G. J.; Jain, A.; Candolfi, C.; Aydemir, U. Chem. Mater. 2021, 33 (5), 1832–1841. https://doi.org/10.1021/acs.chemmater.0c04839.
15. **IFermi: A Python Library for Fermi Surface Generation and Analysis**
    Ganose, A.; Searle, A.; Jain, A.; Griffin, S. JOSS 2021, 6 (59), 3089. https://doi.org/10.21105/joss.03089.
16. **A Simple Model for the Entropy of Melting of Monatomic Liquids**
    Lilley, D.; Jain, A.; Prasher, R. Appl. Phys. Lett. 2021, 118 (8), 083902. https://doi.org/10.1063/5.0041604.
17. **Nondestructive Characterization of Antireflective Coatings on PV Modules**
    Karin, T.; Miller, D.; Jain, A. IEEE J. Photovoltaics 2021, 11 (3), 760–769. https://doi.org/10.1109/JPHOTOV.2021.3053482.

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Pan, H.; Ganose, A. M.; Horton, M.; Aykol, M.; Persson, K. A.; Zimmermann, N. E. R.; Jain, A. Inorg. Chem. 2021, 60 (3), 1590–1603. https://doi.org/10.1021/acs.inorgchem.0c02996.

19. **Experimental Validation of High Thermoelectric Performance in RECuZnP 2 Predicted by High-Throughput DFT Calculations**
Pöhls, J.-H.; Chanakian, S.; Park, J.; Ganose, A. M.; Dunn, A.; Friesen, N.; Bhattacharya, A.; Hogan, B.; Bux, S.; Jain, A.; Mar, A.; Zevalkink, A. Mater. Horiz. 2021, 8 (1), 209–215. https://doi.org/10.1039/D0MH01112F.

20. **Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of Na3V2(PO4)2F3**
Mattei, G. S.; Dagdelen, J. M.; Bianchini, M.; Ganose, A. M.; Jain, A.; Suard, E.; Fauth, F.; Masquelier, C.; Croguennec, L.; Ceder, G.; Persson, K. A.; Khalifah, P. G. Chem. Mater. 2020, 32 (20), 8981–8992. https://doi.org/10.1021/acs.chemmater.0c03190.

21. **A Critical Examination of Compound Stability Predictions from Machine-Learned Formation Energies**
Bartel, C. J.; Trewartha, A.; Wang, Q.; Dunn, A.; Jain, A.; Ceder, G. npj Comput Mater 2020, 6 (1), 97. https://doi.org/10.1038/s41524-020-00362-y.

22. **Benchmarking materials property prediction methods: the Matbench test set and Automatminer reference algorithm**
Dunn, A., Wang, Q., Ganose, A., Dopp, D. & Jain, A. npj Comput Mater 6, 138 (2020).

23. **High Thermoelectric Performance and Defect Energetics of Multipocketed Full Heusler Compounds**
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Spotte-Smith, E. W. C., Yu, P., Blau, S. M., Prasher, R. S. & Jain, A. J Comput Chem 41, 2137–2150 (2020).

25. **Local structure order parameters and site fingerprints for quantification of coordination environment and crystal structure similarity**
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Gorai, P., Ganose, A., Faghaninia, A., Jain, A. & Stevanović, V. Mater. Horiz. 10.1039.D0MH00197J (2020)

27. **Machine Learning Chemical Guidelines for Engineering Electronic Structures in Half-Heusler Thermoelectric Materials**
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28. **Photovoltaic String Sizing Using Site-Specific Modeling**
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29. **An automatically curated first-principles database of ferroelectrics**
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Jordan, D. C., Luo, W., Jain, A., Saleh, M. U., von Korff, H., Hu, Y., Jaubert, J.-N., Mavromatakis, F., Deline, C., Deceglie, M. G., Nag, A., Kimball, G. M., Shinn, A. B., John, J. J., Alnuaimi, A. A. & Elnosh, A. B. A. IEEE J. Photovoltaics 10, 206–212 (2020).

33. **Named Entity Recognition and Normalization Applied to Large-Scale Information Extraction from the Materials Science Literature**
    Weston, L., Tshitoyan, V., Dagdelen, J., Kononova, O., Trewartha, A., Persson, K. A., Ceder, G. & Jain, A. J. Chem. Inf. Model. (2019)
34. **Robocrystallographer: automated crystal structure text descriptions and analysis**
    A.M. Ganose & A. Jain. MRS Communications (2019).
35. **Revelation of Inherently High Mobility Enables Mg3Sb2 as a Sustainable Alternative to n-Bi2Te3 Thermoelectrics**
    X. Shi, C. Sun, Z. Bu, X. Zhang, Y. Wu, S. Lin, W. Li, A. Faghaninia, A. Jain, & Y. Pei. Advanced Science (2019), 1802286
36. **Unsupervised word embeddings capture latent knowledge from materials science literature**
    V.Tshitoyan, J. Dagdelen, L. Weston, A. Dunn, Z. Rong, O. Kononova, K.A. Persson, G. Ceder, & A. Jain. Nature 571, 95–98 (2019).
37. **Automatic Detection of Clear-Sky Periods From Irradiance Data**
    B.H. Ellis, M. Deceglie, & A. Jain. IEEE Journal of Photovoltaics 998 - 1005 (2019).
38. **New horizons in thermoelectric materials: Correlated electrons, organic transport, machine learning, and more**
    J.J. Urban, A.K. Menon, Z. Tian, A. Jain, & K. Hippalgaonkar. Journal of Applied Physics 125, 180902 (2019).
39. **Enhanced Thermochemical Heat Capacity of Liquids: Molecular to Macroscale Modeling**
    P. Yu, A. Jain, & R.S. Prasher. Nanoscale and Microscale Thermophysical Engineering 0, 1–12 (2019).
40. **Rocketsled: a software library for optimizing high-throughput computational searches** A. Dunn, J. Brenneck, & A. Jain. J. Phys. Mater. 2, 034002 (2019).
41. **Origins of ultralow thermal conductivity in 1-2-1-4 quaternary selenides**
    J. Jiahong Kuo, U. Aydemir, J.-H. Pöhls, F. Zhou, G. Yu, A. Faghaninia, F. Ricci, M.A. White, G.-M. Rignanese, G. Hautier, A. Jain, & G.J. Snyder, Journal of Materials Chemistry A 7, 2589–2596 (2019).
42. **Assessing High-Throughput Descriptors for Prediction of Transparent Conductors**
    R. Woods-Robinson, D. Broberg, A. Faghaninia, A. Jain, S.S. Dwaraknath, & K.A. Persson. Chem. Mater. 30, 8375–8389 (2018).
43. **First-principles calculations and experimental studies of XYZ2 thermoelectric compounds: detailed analysis of van der Waals interactions**
    J.-H. Pöhls, Z. Luo, U. Aydemir, J.-P. Sun, S. Hao, J. He, I.G. Hill, G. Hautier, A. Jain, et al., J. Mater. Chem. A. 6, 19502–19519 (2018).
44. **Harnessing the Materials Project for machine-learning and accelerated discovery**
    W. Ye, C. Chen, S. Dwaraknath, A. Jain, S.P. Ong, K.A. Persson, MRS Bull. 43 (2018) 664–669.
45. **The 2019 Materials by Design Roadmap**
    K. Alberi, M.B. Nardelli, A. Zakutayev, L. Mitas, S. Curtarolo, A. Jain, et al., / J. Phys. D. Appl. Phys. 52 (2019) 013001
46. **Matminer: An open source toolkit for materials data mining**
    Logan Ward, Alexander Dunn, Alireza Faghaninia, Nils ER Zimmermann, Saurabh Bajaj, Qi Wang, Joseph Montoya, Jiming Chen, Kyle Bystrom, Maxwell Dylla, Kyle Chard, Mark Asta, Kristin A Persson, G Jeffrey Snyder, Ian Foster, Anubhav Jain / Computational Materials Science 152 (2018) 60-69
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    Juan Li, Xinyue Zhang, Zhiwei Chen, Siqi Lin, Wen Li, Jiahong Shen, Ian T Witting, Alireza Faghaninia, Yue Chen, Anubhav Jain, Lidong Chen, G Jeffrey Snyder, Yanzhong Pei / Joule vol 2, 5 976-987 (2018)
48. **Predicting the volumes of crystals**
    IH Chu, S Roychowdhury, D Han, A Jain, SP Ong / Computational Materials Science 146 (2018) 184–192

49. **Promising thermoelectric performance in van der Waals layered SnSe2**
Yixuan Wu, Wen Li, Alireza Faghaninia, Zhiwei Chen, Juan Li, Xinyue Zhang, Bo Gao, Siqi Lin, Binqiang Zhou, Anubhav Jain, Yanzhong Pei / Materials Today Physics 3, 127-136 (2017)

50. **Assessing local structure motifs using order parameters for motif recognition, interstitial identification, and diffusion path characterization**
NER Zimmermann, MK Horton, A Jain, M Haranczyk / Front. Mater. 4: 34. (2017)

51. **Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows**
Kiran Mathew, Joseph H Montoya, Alireza Faghaninia, Shyam Dwarakanath, Muratahan Aykol, Hanmei Tang, Iek-heng Chu, Tess Smidt, Brandon Bocklund, Matthew Horton, John Dagdelen, Brandon Wood, Zi-Kui Liu, Jeffrey Neaton, Shyue Ping Ong, Kristin Persson, Anubhav Jain / Computational Materials Science 139, 140-152 (2017)

52. **Computational Design of New Magnesium Electrolytes with Improved Properties**
X Qu, Y Zhang, NN Rajput, A Jain, E Maginn, KA Persson / The Journal of Physical Chemistry C 121 (30), 16126-16136 (2017)

53. **An ab initio electronic transport database for inorganic materials**
F Ricci, W Chen, U Aydemir, GJ Snyder, GM Rignanese, A Jain, G Hautier / Scientific data 4, 170085 (2017)

54. **Effective mass and Fermi surface complexity factor from ab initio band structure calculations**
ZM Gibbs, F Ricci, G Li, H Zhu, K Persson, G Ceder, G Hautier, A Jain, GJ Snyder / npj Computational Materials 3 (1), 8 (2017)

55. **Metal phosphides as potential thermoelectric materials**
Jan-Hendrik Pöhls, Alireza Faghaninia, Guido Petretto, Umut Aydemir, Francesco Ricci, Guodong Li, Max Wood, Saneyuki Ohno, Geoffroy Hautier, G Jeffrey Snyder, Gian-Marco Rignanese, Anubhav Jain, Mary Anne White / Journal of Materials Chemistry C 5 (47), 12441-12456 (2017)

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Alireza Faghaninia, Guodong Yu, Umut Aydemir, Max Wood, Wei Chen, Gian-Marco Rignanese, G Jeffrey Snyder, Geoffroy Hautier, Anubhav Jain/ Physical Chemistry Chemical Physics 19 (9), 6743-6756 (2017)

57. **YCuTe2: a member of a new class of thermoelectric materials with CuTe 4-based layered structure**
Umut Aydemir, Jan-Hendrik Pöhls, Hong Zhu, Geoffroy Hautier, Saurabh Bajaj, Zachary M Gibbs, Wei Chen, Guodong Li, Saneyuki Ohno, Danny Broberg, Stephen Dongmin Kang, Mark Asta, Gerbrand Ceder, Mary Anne White, Kristin Persson, Anubhav Jain, G Jeffrey Snyder / Journal of Materials Chemistry A 4 (7), 2461-2472 (2016)

58. **Evaluation of sulfur spinel compounds for multivalent battery cathode applications**
M Liu, A Jain, Z Rong, X Qu, P Canepa, R Malik, G Ceder, KA Persson / Energy & Environmental Science 9 (10), 3201-3209 (2016)

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Wei Chen, Jan-Hendrik Pöhls, Geoffroy Hautier, Danny Broberg, Saurabh Bajaj, Umut Aydemir, Zachary M Gibbs, Hong Zhu, Mark Asta, G Jeffrey Snyder, Bryce Meredig, Mary Anne White, Kristin Persson, Anubhav Jain/ Journal of Materials Chemistry C 4 (20), 4414-4426 (2016) ***invited paper**

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de Jong, Maarten and Chen, Wei and Notestine, Randy and Persson, Kristin and Ceder, Gerbrand and

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62. **Large scale computational screening and experimental discovery of novel materials for high temperature CO_2 capture**
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63. **The Energy Scale of Inorganic Crystalline Metastability**
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68. **Supramolecular Perylene Bisimide-Polysulfide Gel Networks as Nanostructured Redox Mediators in Dissolved Polysulfide Lithium-Sulfur Batteries**
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75. **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), 97, 209-215

76. **Spinel Compounds as Multivalent Battery Cathodes: A Systematic Evaluation Based on *ab initio* Calculations**
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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) 1 (1), 011002 ***invited paper *one of the highest cited papers in the journal's history *cover article** ***equal contributions*
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Jain A., Castelli I. E., Hautier G., Bailey D. H., Jacobsen K. W. / . Materials Science (2013) Volume 48, Issue 19, pp 6519-6534
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Hautier G., Jain A., Mueller T., Moore C., Ong S.P., Ceder G. / Chemistry of Materials (2013) 25 (10), 2064-2074
81. **Improved Capacity Retention for $LiVO_2$ by Cr Substitution**
Ma X., Hautier G., Jain A., Doe R., Ceder G. / J. Electrochemical Society (2012) 160 (2), A279-A284
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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) 68, 314-319
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Ong S.P., Chevrier V.L., Hautier G., Jain A., Moore C.J., Kim S., Ma X., Ceder G. / Energy & Env. Sci. (2011) 4 (9), 3680-3688

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Hautier G., Jain A., Ong S.P., Kang B.W., Moore C., Doe R., Ceder G / Chemistry of Materials (2011) 23 (15), 3495-3508
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92. **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) 84 (4), 045115
93. **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) 50 (8), 2295-2310 ***one of the highest cited papers in the journal's history**
94. **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) 158 (3), A309-A315
95. **Data-mined Ionic Substitution for New Compound Discovery**
Hautier G., Fischer C.C., Erlacher V., Jain A., Ceder G. / Inorganic Chemistry (2011) 50 (2), 656-663
96. **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) 22 (12), 3762-3767
97. **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) 12 (3), 427-430
98. **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) 65 (10), 3025-3033
99. **Are you Centered? An Automatic Crystal-Centering Method for High-Throughput Macromolecular Crystallography**
Jain A., Stojanoff V. / Journal of Synchrotron Radiation (2007) 14 (4), 355-360
100. **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) 18 (2), 23-27

Book chapters

1. **The Materials Project: Accelerating Materials Design through Theory-Driven Data and Tools**
Anubhav Jain, Joseph Montoya, Shyam Dwaraknath, Nils E.R. Zimmermann, John Dagdelen, Matthew Horton, Patrick Huck, Donny Winston, Shreyas Cholia, Shyue Ping Ong, Kristin Persson / *Handbook of Materials Modeling, Springer (2018)*

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.

(utility patent filed August 2010, issued in 2013) US Patent No: US8,399,130 B2 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) US Patent No: US8999282B2
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) US Patent application No: US20140246619A1
5. **Thermal storage and transfer fluids with enhanced specific heat**
   Prasher, R.S., Jain A., Yu, P., Spotte-Smith, E.
   (provisional patent filed April 2019)

10 Selected International Conference Presentations

1. **Software tools for high-throughput materials data generation and data mining**

   TMS Spring, March 2018, *Phoenix, AZ (invited talk)*
2. **Prediction and Experimental Validation of New Bulk Thermoelectrics Compositions from High-Throughput Computations**

   International Conference on Thermoelectrics, August 2017, *Pasadena, CA*
3. **Application of the Materials Project database and data mining towards the design of thermoelectric and functional materials**

   Materials Research Society Fall, Dec 2015, *Boston, MA (invited talk)*
4. **New Energy Storage and Energy Generation Materials from First-Principles Calculations**
   DREAMS workshop, May 2015, *Halifax, Nova Scotia, CA (invited talk)*
5. **The Materials Project: An Electronic Structure Database and its Application to Materials Informatics**
   Materials Research Society, December 2014, *Boston MA (invited talk)*
6. **The Materials Project: An Electronic Structure Database for Community-Based Materials Design**
   ICAMM, July 2014, *Nantes France (invited talk)*
7. **DFT and Materials Informatics: Finding the "needle in the haystack"**
   CAMD Summer School, August 2012, *Lyngby Denmark (invited talk)*
8. **Is it Possible to Design Safe, High-Voltage Cathodes? An Investigation with High-Throughput Computing**
   Electrochemical Society, May 2012, *Seattle WA*
9. **The Materials Genome Project: Using High-Throughput Computing to Design New Materials for Clean Energy**
   CECAM, May 2011, *Lausanne Switzerland (invited talk)*
10. **High-Throughput Materials Design: DFT Calculations on All Reported Crystal Structures And Beyond**
    CECAM, April 2010, *Lausanne Switzerland (invited talk)*

Major awards

- LBL Director's Award, Early Scientific Career (2021)
- Clarivate Highly Cited Researchers (2021)
- DOE Early Career Award (2015)
- NERSC Achievement Award: Innovative Use of High-Performance Computing (2014)
- Luis W. Alvarez Postdoctoral Fellowship (2011)
- DOE Computational Science Graduate Fellowship (2006)
- John McMullen Scholarship (2002)

Selected media

- "Identifying New Materials with NLP with Anubhav Jain". Podcast interview, This Week in Machine Learning (TWiML), https://twimlai.com/podcast/twimlai/identifying-new-materials-nlp-anubhav-jain/
- "Algorithms Uncover Hidden Scientific Knowledge". Media article. https://appliedenergyscience.lbl.gov/news/algorithms-uncover-hidden-scientific
- "AI analyzed 3.3 million scientific abstracts and discovered possible new materials". Media article. https://www.technologyreview.com/2019/07/09/134261/ai-nlp-scientific-abstracts-material-science/

Professional Activities

- co-founder of MaterialsQM Consulting (computational materials design consulting company)
- Associate Director, Materials Project
- Leadership team, DOE DuraMat consortium
- Area lead for "Energy Storage Across Time and Length Scales" (i.e., long duration storage) initiative at LBNL's Energy Technologies area
- Vice President of NERSC User Group Executive Committee (supercomputing center), 2013-2015
- Various mentorship roles (undergraduate research mentor for ~12 students, thesis committee member for ~10 students, part of Computing Sciences mentorship program 2022,)
- Judging panel member for various early career initiatives (LBL postdoc SLAM, materials "hackathons" at MRS Fall 2014 and MRS Fall 2015, NSF workshop on thermal storage).
- Various referee roles (referee for multiple journals, Argonne Center for Nanoscale Materials proposal evaluation board, commitee to determine LBL ETA Newman fellows)
- Co-created the Materials Project seminar series, which hosts top researchers in materials design for virtual talks (monthly). Typically get ~200 live attendees and ~1000 views on posted videos.
- develop and maintain several open-source software that are widely used by the materials community: FireWorks for running high-throughput calculations at supercomputing centers, atomate for “recipes” of calculation workflows for computing various materials and molecular properties, and matminer for applying data mining to materials

- completed "Good to Great" leadership program (~10 day course)
- maintain a Twitter feed summarizing all my papers (twitter.com/jainpapers)