

John M. Dagdelen

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EDUCATION

University of California, Berkeley

B.S. Materials Science and Engineering (May 2016), M.S. Materials Science and Engineering (May 2019),
Ph.D. Materials Science and Engineering | August 2017 – December 2022 (expected)

RESEARCH AND ENGINEERING EXPERIENCE

Lawrence Berkeley National Laboratory | Berkeley, CA ----- August 2017 – Present
Graduate Student Researcher, Environmental Energy Technologies Division, Persson Group

- Machine learning for materials discovery and design.
- Natural language processing applied to scientific text.
- <http://matscholar.com/>: Materials literature search engine augmented with data extracted from text with NLP, mat2vec word embedding visualization.
- <http://covidscholar.org/>: COVID-19 search engine used by thousands of researchers during the pandemic. Successfully applied for and won LBNL LDRD and \$500k C3.ai DTI grant.

Google Brain | Remote, CA ----- May 2021 – September, 2021
Research Intern, Google Research

- Developed Graph Neural Network (GNN) models estimating the formation energy of amorphous materials at state-of-the-art accuracy, trained on ab initio density functional theory calculations.
- Applied GNN model to predict synthesizability of metastable compounds and discover new inorganic crystalline compounds.

Lawrence Berkeley National Laboratory | Berkeley, CA ----- October 2015 – August 2017
Research Associate, Environmental Energy Technologies Division, Persson Group

- High-throughput DFT-based screening for materials with exotic mechanical properties which identified 8 novel auxetic crystalline materials (only 1 previously known to science prior.)

National Renewable Energy Laboratory | Golden, CO ----- Summer 2015
DOE Science Undergraduate Laboratory Intern (SULI), Chemistry and Nanoscience

- Investigated mechanisms of perovskite solar cell degradation and developed solution-based nanocomposite coatings that increase lifetime of perovskite films 50x. Patent awarded November 2020.

National Renewable Energy Laboratory | Golden, CO ----- Summer 2014
Intern, Concentrating Solar Power Group

- Developed high-temperature silica sol-gel oxidation barrier coatings for Concentrating Solar Power (CSP) receiver systems.

NSF REU, Colorado School of Mines | Golden, CO ----- Summer 2013
Department of Metallurgy and Materials Science, Advanced Steel Processing and Products Research Center

- Investigated and characterized fatigue properties of advanced high strength steel alloys to enable safer, more fuel efficient, and less expensive manufacture of car bodies.
 - XRD and SEM microstructure analysis to measure stability of retained austenite during fatigue testing.
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SKILLS & TECHNOLOGIES

- **Languages:** Python, Javascript, C, C++, Matlab
 - **Machine Learning Libraries:** Jax, Haiku, Jraph, PyTorch, TensorFlow
 - **Other Frameworks and Tools:** MongoDB, Vespa.ai, React, FastAPI, Flask
 - **Natural Language Understanding and Machine Learning** (including graduate level coursework): language modeling, word embeddings, named entity recognition, deep reinforcement learning, and some computer vision
 - **High Throughput Density Functional Theory:** VASP, Atomate, FireWorks, Pymatgen
 - **Parallel Computing** (including graduate level coursework): OpenMP, MPI, CUDA
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PUBLICATIONS AND PATENTS

[Algorithms for Materials Discovery](#). Dagdelen, J. and Dunn, A. Chapter in *Accelerated Materials Discovery: How to Use Artificial Intelligence to Speed Up Development*. Walter de Gruyter GmbH & Co KG. (2022)

[The Impact of Domain-Specific Pre-Training on Named Entity Recognition Tasks in Materials Science](#)

Walker, N., Trewartha, A., Huo, H., Lee, S., Cruse, K., Dagdelen, J., Dunn, A., Persson, K., Ceder, G., and Jain, A. *Patterns*. 3(4), 100488. (2021)

[Online Interactive Platform for COVID-19 Literature Visual Analytics](#). Moran et al. - *Journal of Medical Internet Research*. 23 (7), e26995 (2021)

[Nanocomposite coatings for perovskite solar cells and methods of making the same](#)

Zhu, K., Ma Z., Dagdelen, J. - US Patent 10,847,738. (2020)

[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. *Journal of Chemical Information and Modeling*, 59(9), 3692–3702. (2019)

[COVIDScholar: An automated COVID-19 research aggregation and analysis platform](#). A Trewartha, J Dagdelen, H Huo, K Cruse, Z Wang... - arXiv preprint arXiv:2012.03891. (2020)

[Enumeration as a Tool for Structure Solution: A Materials Genomic Approach to Solving the Cation-Ordered Structure of Na₃V₂\(PO₄\)₂F₃](#). GS Mattei, JM Dagdelen, et al. *Chemistry of Materials*, (2020)

[Unsupervised word embeddings capture latent knowledge from materials science literature](#). Tshitoyan, V., Dagdelen, J., Weston, L., Dunn, A., Rong, Z., Kononova, O., Persson, K. A., Ceder, G., Jain, A. *Nature*. 571(7763), 95-98. (2019)

[“The Materials Project: Accelerating Materials Design Through Theory-Driven Data and Tools”](#) in *Handbook of Materials Modeling*. Jain, A., Montoya, J., Dwaraknath, S., Zimmermann, N. E., Dagdelen, J., Horton, M., ... Ong, S. P.; Springer, Cham. (2018)

[Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows](#). Mathew, K., et al. *Computational Materials Science*, 139, 140–152. (2017)

[Computational Prediction of New Auxetic Materials](#). Dagdelen, J., Montoya, J., de Jong, M., Persson, K. *Nature Communications*. 8(1), 323 (2017)

[Application of Sol-Gel Method as a Protective Layer on a Specular Reflective Surface for Secondary Reflector in a Solar Receiver](#). Afrin, S., Dagdelen, J., Ma, Z., & Kumar, V. *Proceedings of the ASME 2016 10th International Conference on Energy Sustainability*. (2016)

LECTURES, PRESENTATIONS, AND POSTERS

“Matscholar: A search engine for materials science research” Berlin Buzzwords 2022, Berlin, Germany. June 2022

CoDA 2020. (Winner, best poster). Santa Fe, NM. February 2020.

“Natural Language Processing for Materials Discovery and Design” (Invited Talk) IEEE MetroCon. Dallas-Fort Worth, TX. October 2019

“Adapting Natural Language Processing Methods to Materials Research” (Invited Talk) NERSC Data Seminar. Lawrence Berkeley National Laboratory. Berkeley, CA. December 6, 2019

“Driving Materials Innovation with Natural Language Processing” (Invited Talk, Keynote) National Research Council Workshop on Artificial Intelligence for Design. Ottawa, Canada. November 2019

“Natural Language Processing for Materials Discovery and Design” (Poster) Materials Research Society Spring Meeting. Phoenix, AZ. April 2018 (nominated for best poster)

“Guiding Materials Design with Unsupervised Machine Learning Methods” (Talk) Materials Research Society Fall Meeting. Boston, MA. November 2018

“Natural Language Processing for Materials Discovery.” (Talk) Machine Learning for Science. Lawrence Berkeley National Laboratory. Berkeley, CA. September 2018

“Computational Investigation of Poisson’s Ratio and its Relationship to Crystal Structure.” (Talk) American Crystallographic Association Annual Meeting. Toronto, Canada. July 2018

“Extracting Materials Knowledge from Text Using Artificial Intelligence.” (Poster) Toyota Research Institute Advanced Materials Design and Discovery Workshop. San Francisco, CA. June 2018

“Review of Energy Generation Trends in the United States.” (Keynote) International Energy Raw Materials and Energy Summit. Istanbul Technical University. Istanbul, Turkey. September 2017

“Accessing Materials Project Data Through the Materials API (MAPI).” (Workshop Session) Materials Project Workshop. University of California, Berkeley. Berkeley, CA. August 2017, 2018, 2019

“Organic-Inorganic Hybrid Nanocomposite Coatings for High-Stability Perovskite Solar Cells.” (Poster, 2nd place) Science Undergraduate Laboratory Internship (SULI) poster competition. National Renewable Energy Laboratory (NREL). Golden, CO. July 2015

ACTIVITIES AND ASSOCIATIONS

University of California, Berkeley Innovation & Entrepreneurship Council | UC Berkeley

Computer Science Graduate Entrepreneurship Council | UC Berkeley

Computational Materials at Berkeley | UC Berkeley Registered Student Org., *President*

Kavli Energy Nanoscience Institute | UC Berkeley College of Engineering, *Faculty Group Representative*

MSE Graduate Student Council | UC Berkeley, *1st Year Representative (2017-2018), Vice President (2018-2019)*

Graduate Assembly | UC Berkeley Graduate Assembly, *MSE Department Alternate Representative*

AWARDS

- UC Berkeley **Outstanding Graduate Student Instructor Award** (2020)
- **Best Poster** CoDA 2020 (Conference on Data Analysis, awarded by American Statistical Association)
- UC Berkeley **Elaine Shen Memorial Prize**
- Chi Phi Educational Trust Graduate Scholarship
- Best Poster (nominated) Materials Research Society Spring Meeting (2019)
- **Dean’s Honors**, Spring 2015, Fall 2016
- 2nd Place, **NREL SULI Poster Competition**, Summer 2015