

Arun Mannodi Kanakkithodi, Ph.D.

Summary of Qualifications

- Computational material scientist with 7+ years of experience in density functional theory, ab initio molecular dynamics and machine learning
- Interdisciplinary collaborator with experience in guided experimental discovery of energy materials and applying data science and learning to materials data
- Author of 25+ publications in peer-reviewed journals, including 4 invited reviews
- Co-developer of Polymer Genome (<http://polymergenome.org/>), an informatics platform for property prediction of polymers

Education

- 2012–2017 **Ph.D. Materials Science and Engineering**, University of Connecticut, Storrs, CT, USA, *Dissertation: Rational Design of Polymer Dielectrics via First Principles Computations and Machine Learning*, Supervisor: Prof. Rampi Ramprasad
GPA: 3.956/4
- 2008–2012 **Bachelor of Technology, Metallurgical and Materials Engineering**, Indian Institute of Technology (IIT) Roorkee, Roorkee, Uttarakhand, India
GPA: 7.807/10

Experience

- June 2017 – Present **Postdoctoral Researcher**, ARGONNE NATIONAL LABORATORY, Lemont, IL, USA
Tuning the electronic and defect properties of semiconductors using first principles computations
- Developed first of its kind comprehensive computational database of defect properties of halide perovskites and semiconductors belonging to groups IV, III-V and II-VI
 - Trained machine learning models to learn chemical patterns and design rules for semiconductors with tailored impurity levels, driving experimental discovery of novel solar cell absorbers
 - Studied the structure and infrared spectra of crystalline, cross-linked and moisture containing solar cell encapsulant polymers to aid the experimental understanding of the effect of moisture in solar cell modules
 - Successfully executed research proposals to secure several million core hours of computational time at XSEDE, NERSC, and Argonne resources
- August 2012 – May 2017 **Graduate Research Assistant**, UNIVERSITY OF CONNECTICUT, Storrs, CT, USA
Rational design of polymer dielectrics using density functional theory and machine learning
- Executed thousands of density functional theory computations that led to the identification of several novel dielectric polymer candidates for high energy density capacitors
 - Developed machine learning based on-demand predictive models that allowed expansion of knowledge to previously unexplored polymer chemical spaces
 - Collaborated with experimental chemists to lead the discovery of all new organic and organometallic polymers with attractive dielectric and electronic properties
- February 2015 – **Research Internship**, LOS ALAMOS NATIONAL LABORATORY, Los Alamos, New Mexico, USA
Multi-objective optimization of polymers with attractive dielectric properties
- Collaborated with scientists in the theory and computing divisions to apply machine learning on computational data, optimize polymer compositions for targeted combination of properties
 - Wrote a substantial number of lines of code in Python to implement machine learning techniques like ridge regression, support vector regression, random forest regression and efficient global optimization.
- August 2013 – May 2014 **Teaching Assistant**, UNIVERSITY OF CONNECTICUT, Storrs, CT, USA
Assisted Prof. Theo Kattamis in planning and conducting lectures and grading beginner level materials science graduate and undergraduate courses.

Computational Skills

Programming Python, MATLAB, Git, Linux/UNIX, Shell scripting, FORTRAN, C, L^AT_EX, High Performance Computing
Software Materials modeling (VASP, LAMMPS), Visualization (VMD, Materials Studio), Scikit-learn, NumPy, SciPy, MLPy, Pymatgen

Awards, Scholarships and Honors

- 2016 Graduate Student Silver Award, Materials Research Society
- 2016 Graduate Student of the Year Award, Materials Science and Engineering, University of Connecticut
- 2016 Ovshinsky Student Travel Award, American Physical Society
- 2016 Best Presenter Award, ASM Hartford Chapter Student Speaking Contest
- 2014 GE Graduate Fellowship for Innovation, University of Connecticut
- 2014 Best Student Oral Presentation Award, Materials Research Society
- 2013 Nominee for Best Poster Presentation, Materials Research Society

Outreach Activities and Service

- 2018 – **Board Member, Postdoctoral Society**, ARGONNE NATIONAL LABORATORY
Present Co-organized social, educational and career-oriented events for the postdoc community at Argonne.
- 2018 – **Organizer, Journal Club**, ARGONNE NATIONAL LABORATORY
Present Organized bi-weekly presentations by prominent researchers in the areas of machine learning and high performance computing, attended by a wide audience of Argonne postdocs and scientists.
- April 2016 **Judge at Connecticut Invention Convention**, UNIVERSITY OF CONNECTICUT
Evaluated scientific inventions by Connecticut high school students and mentored a selected group of innovators for the national and international stages.
- 2014 – 2017 **Member, Materials Research Society Student Chapter**, UNIVERSITY OF CONNECTICUT
Co-organized social, educational and career-oriented events for the materials science and engineering graduate student community at UConn.

Publications

Published Journal Articles

- 2019 26. **A. Mannodi-Kanakkithodi**, J. S. Park, N. Jeon, D. H. Cao, D. J. Gosztola, A. B. F. Martinson, M. K. Y. Chan, "Comprehensive Computational Study of Partial Lead Substitution in Methylammonium Lead Bromide", *Chemistry of Materials* 31 (10), 3599–3612 (2019).
- 2019 25. Q. Shao, **A. Mannodi-Kanakkithodi**, Y. Xia, M. K. Y. Chan, M. Grayson, "Seebeck Tensor Analysis of (p × n)-type Transverse Thermoelectric Materials", *MRS Advances* 4 (8), 491–497 (2019).
- 2019 24. D. H. Cao, P. Guo, **A. Mannodi-Kanakkithodi** G. P. Wiederrecht, D. J. Gosztola, N. Jeon, R. D. Schaller, M. K. Y. Chan, A. B. F. Martinson, "Charge Transfer Dynamics of Phase Segregated Halide Perovskites: CH₃NH₃PbCl₃ and CH₃NH₃PbI₃ or (C₄H₉NH₃)₂(CH₃NH₃)_{n-1}Pb_nI_{3n+1} mixtures", *ACS Appl. Mater. Interfaces* 11, 9583–9593 (2019).
- 2019 23. P. Guo, **A. Mannodi-Kanakkithodi**, J. Gong, Y. Xia, C. C. Stoumpos, D. H. Cao, B. T. Diroll, J. B. Ketterson, G. P. Wiederrecht, T. Xu, M. K. Y. Chan, M. G. Kanatzidis, R. D. Schaller "Infrared-pump electronic-probe of methylammonium lead iodide reveals electronically decoupled organic and inorganic sublattices", *Nature Communications* 10, 482 (2019).
- 2018 22. BOOK CHAPTER: **A. Mannodi-Kanakkithodi**, R. Ramprasad, "Rational Design of Polymer Dielectrics: An Application of Density Functional Theory and Machine Learning", *Computational Materials Discovery*, The Royal Society of Chemistry (2018).
- 2018 21. INVITED REVIEW: **A. Mannodi-Kanakkithodi**, A. Chandrasekaran, C. Kim, T. D. Huan, G. Pilania, V. Botu, R. Ramprasad, "Scoping the Polymer Genome: A Roadmap for Rational Polymer Dielectrics Design and Beyond", *Materials Today* 1369-7021 (2018).

- 2018 20. S. Nasreen, G. M. Treich, M. L. Baczkowski, **A. Mannodi-Kanakkithodi**, A. F. Baldwin, S. K. Scheirey, Y. Cao, R. Ramprasad, G. A. Sotzing, "A Material Genome Approach towards Exploration of Zn- and Cd-Coordination Complex Polyester as Dielectrics: Design, Synthesis and Characterization", *Polymer* in press (2018).
- 2017 19. INVITED REVIEW: R. Ramprasad, R. Batra, G. Pilia, **A. Mannodi-Kanakkithodi**, C. Kim, "Machine Learning and Materials Informatics: Recent Applications and Prospects", *npj Computational Materials* 3, 54 (2017).
- 2017 18. BOOK CHAPTER: J. Hill, **A. Mannodi-Kanakkithodi**, R. Ramprasad, B. Meredig, "Materials Data Infrastructure and Materials Informatics", *Computational Materials System Design*, Springer International Publishing (2017).
- 2017 17. BOOK CHAPTER: S. Nasreen, G. M. Treich, M. L. Baczkowski, **A. Mannodi-Kanakkithodi**, Y. Cao, R. Ramprasad, G. Sotzing, "Polymer Dielectrics for Capacitor Application", *Kirk-Othmer Encyclopedia of Chemical Technology*, John Wiley & Sons, Inc (Ed.) (2017).
- 2017 16. **A. Mannodi-Kanakkithodi**, T. D. Huan, R. Ramprasad, "Mining materials design rules from data: The example of polymer dielectrics", *Chemistry of Materials* 29 (21), 9001 (2017).
- 2017 15. G. Pilia, **A. Mannodi-Kanakkithodi**, "First-principles identification of novel double perovskites for water-splitting applications", *Journal of Materials Science* 52 (14), 8518 (2017).
- 2017 14. S. Biswas, B. Dutta, **A. Mannodi-Kanakkithodi**, R. Clarke, W. Song, R. Ramprasad, S. L. Suib, "Heterogeneous Mesoporous Manganese/Cobalt Oxide Catalyst for Selective Oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran", *Chemical Communications* 53, 11751 (2017).
- 2017 13. G. M. Treich, M. Tefferi, S. Nasreen, **A. Mannodi-Kanakkithodi**, Z. Li, R. Ramprasad, G. A. Sotzing, Y. Cao, "A rational co-design approach to the creation of new dielectric polymers with high energy density", *IEEE Transactions on Dielectrics and Electrical Insulation* 24, 732 (2017).
- 2016 12. G. M. Treich, S. Nasreen, **A. Mannodi-Kanakkithodi**, R. Ma, M. Tefferi, J. Flynn, Y. Cao, R. Ramprasad, G. A. Sotzing, "Optimization of Organotin Polymers for Dielectric Applications", *ACS Applied Materials and Interfaces* 8 (33), 21270 (2016).
- 2016 11. **A. Mannodi-Kanakkithodi**, G. Pilia, R. Ramprasad, "Critical assessment of regression-based machine learning methods for polymer dielectrics", *Computational Materials Science* 125, 123 (2016).
- 2016 10. **A. Mannodi-Kanakkithodi**, G. Pilia, R. Ramprasad, T. Lookman, J.E. Gubernatis, "Multi-objective optimization techniques to design the Pareto front of organic dielectric polymers", *Computational Materials Science* 125, 92 (2016).
- 2016 9. M. Misra, **A. Mannodi-Kanakkithodi**, T. C. Chung, R. Ramprasad, S. K. Kumar, "Critical role of morphology on the dielectric constant of semicrystalline polyolefins", *Journal Chemical Physics* 144, 234905 (2016).
- 2016 8. **A. Mannodi-Kanakkithodi**, G. M. Treich, T. D. Huan, R. Ma, M. Tefferi, Y. Cao, G. A. Sotzing, R. Ramprasad, "Rational Co-Design of Polymer Dielectrics for Energy Storage", *Advanced Materials* 28, 6277 (2016).
- 2016 7. T. D. Huan, **A. Mannodi-Kanakkithodi**, C. Kim, V. Sharma, G. Pilia, R. Ramprasad, "A polymer dataset for accelerated property prediction and design", *Scientific Data* 3, 160012 (2016).
- 2016 6. **A. Mannodi-Kanakkithodi**, G. Pilia, T. D. Huan, T. Lookman, R. Ramprasad, "Machine Learning Strategy for Accelerated Design of Polymer Dielectrics", *Scientific Reports* 6, 20952 (2016).
- 2016 5. G. Pilia, **A. Mannodi-Kanakkithodi**, B. P. Uberuaga, R. Ramprasad, J. E. Gubernatis, T. Lookman, "Machine learning bandgaps of double perovskites", *Scientific Reports* 6, 19375 (2016).
- 2015 4. T. D. Huan, **A. Mannodi-Kanakkithodi**, R. Ramprasad, "Accelerated materials property predictions and design using motif-based fingerprints", *Physical Review B*. 92, 014106 (2015).
- 2015 3. A. F. Baldwin, T. D. Huan, R. Ma, **A. Mannodi-Kanakkithodi**, M. Tefferi, J. E. Marszalek, N. Katz, Y. Cao, R. Ramprasad, G. A. Sotzing, "Rational Design of Organotin Polyesters", *Macromolecules* 48, 2422 (2015).
- 2015 2. A. F. Baldwin, R. Ma, **A. Mannodi-Kanakkithodi**, T. D. Huan, C. C. Wang, M. Tefferi, J. E. Marszalek, M. Cakmak, Y. Cao, R. Ramprasad, G. A. Sotzing, "Poly(dimethyltin glutarate) as a Prospective Material for High Dielectric Applications", *Advanced Materials* 27, 346 (2015).

- 2015 1. **A. Mannodi-Kanakkithodi**, C.C. Wang, R. Ramprasad, "Compounds based on Group 14 elements: building blocks for advanced insulator dielectrics design", *Journal of Materials Science* 50, 801 (2015).

Upcoming Journal Articles

- 2019 1. **A. Mannodi-Kanakkithodi**, M. Toriyama, F. G. Sen, M. Davis, R. F. Klie, M. K. Y. Chan, "Machine learned impurity level prediction in semiconductors: the example of Cd-based chalcogenides", *under review*, preprint: arXiv:1906.02244.
- 2019 2. **A. Mannodi-Kanakkithodi**, J. S. Park, A. B. F. Martinson, M. K. Y. Chan, "Defect Physics of Pseudo-cubic Mixed Halide Lead Perovskites from First Principles", *under review*.
- 2019 3. F. G. Sen, **A. Mannodi-Kanakkithodi**, T. Paulauskas, J. Guo, L. Wang, A. Rockett, M. J. Kim, R. F. Klie, M. K. Y. Chan, "Computational Design of Passivants for CdTe Grain Boundaries", *under review*.
- 2019 4. J. Guo, F. G. Sen, **A. Mannodi-Kanakkithodi**, M. J. Kim, M. K. Y. Chan, E. Barnard, W. Sampath, R. F. Klie, "Effect of Se and Cl segregation in polycrystalline CdSeTe devices", *under review*.
- 2019 5. E. Schwenker, **A. Mannodi-Kanakkithodi**, F. G. Sen, S. Hills, M. K. Y. Chan, "Inversion of Atomic-Resolution CdTe Grain Boundary Images Using Atomistic Simulation and Computer Vision", to be submitted.
- 2019 6. B. T. Diroll, **A. Mannodi-Kanakkithodi**, M. K. Y. Chan, R. D. Schaller, "Spectroscopic Comparison of Thermal Transport at Organic-Inorganic and Organic-Hybrid Interfaces: CsPbBr₃ and FAPbBr₃ Perovskite Nanocrystals", to be submitted.
- 2019 7. **A. Mannodi-Kanakkithodi**, R. E. Kumar, D. P. Fenning, M. K. Y. Chan, "First Principles Modeling of Water-induced Polymer Encapsulant Degradation in Silicon Modules", to be submitted.

Conference Proceedings and Presentations

Published Proceedings

- 2018 1. **A. Mannodi-Kanakkithodi**, J-S. Park, D. H. Cao, N. Jeon, A. B. F. Martinson, M. K. Y. Chan, "First-principles Study of Intrinsic and Extrinsic Point Defects in Lead-Based Hybrid Perovskites", *45th IEEE Photovoltaic Specialists Conference* 0495-0498 (2018).
- 2018 2. F. G. Sen, **A. Mannodi-Kanakkithodi**, T. Paulauskas, C. Sun, J. Guo, L. Wang, J. Wands, A. Rockett, M. J. Kim, R. F. Klie, M. K. Y. Chan, "Efficient CdTe photovoltaics by co-passivating grain boundaries", *45th IEEE Photovoltaic Specialists Conference* 3880-3883 (2018).

Oral and Poster Presentations

- 2019 40. Oral: **A. Mannodi-Kanakkithodi**, M. Toriyama, F. G. Sen, M. Davis, R. F. Klie, M. K. Y. Chan, "Machine-learned impurity level prediction in semiconductors: the example of Cd-based chalcogenides", Session: Advanced Characterization and Simulation of CdTe, *46th IEEE Photovoltaic Specialists Conference*, Chicago, Illinois, June 18 (2019).
- 2019 39. Oral: **A. Mannodi-Kanakkithodi**, M. Toriyama, F. G. Sen, M. Davis, R. F. Klie, M. K. Y. Chan, "Machine-learned impurity level prediction in semiconductors: the example of Cd-based chalcogenides", Materials Science and Engineering Track, *Machine Learning in Science and Engineering*, Atlanta, Georgia, June 10 (2019).
- 2019 38. Oral: **A. Mannodi-Kanakkithodi**, M. Davis, M. K. Y. Chan, "Machine Learned Defect Level Predictor for Cd-Based Chalcogenides", Session: Calculation and Prediction, *Materials Research Society Spring Meeting*, Phoenix, Arizona, April 25 (2019).
- 2019 37. Oral: **A. Mannodi-Kanakkithodi**, D. H. Cao, N. Jeon, J-S. Park, A. B. F. Martinson, M. K. Y. Chan, "Point Defect Engineering in Lead-Based Mixed Halide Hybrid Perovskites via First Principles Computations", Session: First Principles and Computational Screening I, *Materials Research Society Spring Meeting*, Phoenix, Arizona, April 24 (2019).
- 2019 36. Oral: **A. Mannodi-Kanakkithodi**, M. Davis, M.K.Y. Chan, "Machine learned defect level prediction for lead-based hybrid perovskites", Symposium: Computational Materials Discovery and Design, *The Minerals, Metals and Materials Society Meeting*, San Antonio, Texas, March 12 (2019).
- 2019 35. Oral: **A. Mannodi-Kanakkithodi**, E. Schwenker, F. G. Sen, L. Chen, S. Hills, J. Guo, M. Kim, R. Klie, M. K. Y. Chan, "Modeling realistic grain boundaries in CdTe", Session K47: Photovoltaics – Solar Energy Conversion I, *American Physical Society March Meeting*, Boston, Massachusetts, March 6 (2019).

- 2019 34. Oral: **A. Mannodi-Kanakkithodi**, D. H. Cao, N. Jeon, J-S. Park, M. Davis, A. B. F. Martinson, M. K. Y. Chan, "Machine learned defect level predictor for semiconductors", Session F16: Computational Materials Design and Discovery – Semiconductors, *American Physical Society March Meeting*, Boston, Massachusetts, March 5 (2019).
- 2018 33. Oral: **A. Mannodi-Kanakkithodi**, M. Davis, M.K.Y. Chan, "Machine Learned Defect Level Predictor for Semiconductors: The Example of Hybrid Perovskites", Symposium: Machine Learning and Data-Driven Materials Development and Design, *Materials Research Society Fall Meeting*, Boston, Massachusetts, November 26 (2018).
- 2018 32. Oral: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Compensation of Intrinsic Point Defects by Extrinsic Substitution in Lead-Based Mixed Halide Hybrid Perovskites", Symposium: Harvesting Functional Defects in Energy Materials, *Materials Research Society Fall Meeting*, Boston, Massachusetts, November 27 (2018).
- 2018 31. Poster: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Tuning the Electronic and Defect Properties of Methylammonium Lead Bromide via Composition Engineering", Session: Fundamentals of Halide Perovskite Optoelectronics II, *Materials Research Society Fall Meeting*, Boston, Massachusetts, November 27 (2018).
- 2018 30. Invited Lecture: **A. Mannodi-Kanakkithodi**, "Computational Modeling of Energy Nanomaterials", Summer School on Nanotechnology for Energy, *IEEE Nanotechnology Materials and Devices Conference*, Portland State University, Portland, Oregon, October 14 (2018).
- 2018 29. Oral: F.G. Sen, **A. Mannodi-Kanakkithodi**, T. Paulauskas, C. Sun, J. Guo, L. Wang, J. Wands, A. Rockett, M.J. Kim, R.F. Klie, M.K.Y. Chan, "Efficient CdTe Photovoltaics by Co-Passivating Grain Boundaries", Session: Material Properties, *World Conference On Photovoltaic Energy Conversion (WCPEC-7)*, Waikoloa, Hawaii, June 15 (2018).
- 2018 28. Poster: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "First Principles Study of Intrinsic and Extrinsic Point Defects in Lead-Based Hybrid Perovskites", Session: Perovskite Materials and Devices, *World Conference On Photovoltaic Energy Conversion (WCPEC-7)*, Waikoloa, Hawaii, June 11 (2018).
- 2018 27. Poster: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Tailoring the Electronic and Defect Properties of Methylammonium Lead Bromide Hybrid Perovskite via Composition Engineering", Symposium: Advances in Perovskite Solar Cell Devices and Applications, *Materials Research Society Spring Meeting*, Phoenix, Arizona, April 4 (2018).
- 2018 26. Oral: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Defect Physics of Lead-Based Mixed Halide Hybrid Perovskites from First Principles Computations", Symposium: Novel Materials Physics of Perovskite Semiconductors, *Materials Research Society Spring Meeting*, Phoenix, Arizona, April 3 (2018).
- 2018 25. Oral: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Intermediate Bands in Hybrid Perovskites", Session A11: Organometal Halide Perovskites I, *American Physical Society March Meeting*, Los Angeles, California, March 5 (2018).
- 2018 24. Invited Talk: **A. Mannodi-Kanakkithodi**, H.D. Tran, C. Kim, R. Ramprasad, "Rational Design of Polymer Dielectrics: An Application of Density Functional Theory and Machine Learning", Session: Data Science and High-Throughput Approaches I, *Conference on Electronic and Advanced Materials*, Orlando, Florida, January 19 (2018).
- 2018 23. Oral: **A. Mannodi-Kanakkithodi**, J.S. Park, D.H. Cao, N. Jeon, A.F. Martinson, M.K.Y. Chan, "Energetics of intrinsic and extrinsic defects in lead-based hybrid perovskites from first principles computations", Session: Defect Physics and Chemistry, *Conference on Electronic and Advanced Materials*, Orlando, Florida, January 18 (2018).
- 2017 22. Oral: S. Nasreen, G.M. Treich, M.L. Baczowski, **A. Mannodi-Kanakkithodi**, Y. Cao, R. Ramprasad, G.A. Sotzing, "A Rational Co-Design Approach for Next Generation Dielectric Materials with the Transition Metal Containing Coordination Polymers", Session: New Materials and Devices, *Electrochemical Society (ECS) Meeting*, National Harbor, Maryland, October 5 (2017).

- 2017 21. Poster: **A. Mannodi-Kanakkithodi**, F.G. Sen, S. Hills, A. Kinaci, B. Narayanan, A. Wey, K. Letchworth-Weaver, S. Gray, S. Sankaranarayanan, M.K.Y. Chan, M. Davis, G. Pilania, R. Ramprasad, H.D. Tran, C. Kim, "Data-driven Design of Functional Materials: Examples of Polymer Dielectrics, Photovoltaic Materials and Nanocatalysts", *Materials Research and Data Science Conference*, NIST/UMD Institute for Bioscience and Biotechnology Research, Rockville, Maryland, September 25 (2017).
- 2017 20. Poster: S. Nasreen, M. Baczowski, G. Treich, **A. Mannodi-Kanakkithodi**, S. Scheirey, R. Ramprasad, G. Sotzing, "Zinc and cadmium coordination polymers of aliphatic systems as dielectric materials", PMSE 411, *American Chemical Society National Meeting*, San Francisco, California, April 4 (2017).
- 2017 19. Oral: S. Scheirey, G. Treich, S. Nasreen, Z. Li, **A. Mannodi-Kanakkithodi**, Y. Cao, R. Ramprasad, G. Sotzing, "Polyureas for dielectric applications developed through a rational co-design approach", POLY 150, *American Chemical Society National Meeting*, San Francisco, California, April 3 (2017).
- 2017 18. Oral: G. Treich, M. Misra, S. Nasreen, M. Tefferi, **A. Mannodi-Kanakkithodi**, R. Ramprasad, Y. Cao, G. Sotzing, "Synthesis, characterization, and analysis of a novel polythiourea for dielectric applications aided by molecular dynamics and density functional theory", POLY 269, *American Chemical Society National Meeting*, San Francisco, California, April 2 (2017).
- 2016 17. Oral: **A. Mannodi-Kanakkithodi**, H. Tran, R. Ramprasad, "Rational Design of Polymer Dielectrics via First Principles Computations and Machine Learning", Session TC1: In-Silico Materials Design, *Materials Research Society Fall Meeting*, Boston, Massachusetts, November 30 (2016).
- 2016 16. Oral: **A. Mannodi-Kanakkithodi**, H.D. Tran, G. Treich, G. Pilania, T. Lookman, G. Sotzing, R. Ramprasad, "Rational Design of Polymer Dielectrics", Session: Clean Energy / Storage / Emerging Technologies, *Connecticut Symposium on Microelectronics and Optoelectronics*, Storrs, Connecticut, April 6 (2016).
- 2016 15. Oral: **A. Mannodi-Kanakkithodi**, H.D. Tran, G. Pilania, T. Lookman, R. Ramprasad, "Rational Co-Design of Polymer Dielectrics for Energy Storage", Session H23: Computational Discovery and Design of Materials for Catalysis, *American Physical Society March Meeting*, Baltimore, Maryland, March 15 (2016).
- 2016 14. Oral: J.E. Gubernatis, **A. Mannodi-Kanakkithodi**, R. Ramprasad, G. Pilania, T. Lookman, "A Multi-Objective Optimization Technique to Model the Pareto Front of Organic Dielectric Polymers", Session E22: Predicting and Classifying Materials via High-Throughput Databases and Machine Learning I, *American Physical Society March Meeting*, Baltimore, Maryland, March 15 (2016).
- 2016 13. Oral: G. Pilania, **A. Mannodi-Kanakkithodi**, B. Uberuaga, R. Ramprasad, J.E. Gubernatis, T. Lookman, "Machine learning bandgaps of double perovskites", Session E22: Predicting and Classifying Materials via High-Throughput Databases and Machine Learning I, *American Physical Society March Meeting*, Baltimore, Maryland, March 15 (2016).
- 2016 12. Oral: H.D. Tran, **A. Mannodi-Kanakkithodi**, C. Kim, V. Sharma, G. Pilania, R. Ramprasad, "A comprehensive polymer dataset for accelerated property prediction and design", Session E22: Predicting and Classifying Materials via High-Throughput Databases and Machine Learning I, *American Physical Society March Meeting*, Baltimore, Maryland, March 15 (2016).
- 2015 11. Oral: **A. Mannodi-Kanakkithodi**, G. Pilania, H.D. Tran, T. Lookman, R. Ramprasad, "On-Demand Data-Driven Design of Organic Dielectric Polymers", Symposium CCC: Integrating Experiments, Simulations and Machine Learning to Accelerate Materials Innovation, *Materials Research Society Fall Meeting*, Boston, Massachusetts, December 1 (2015).
- 2015 10. Oral: **A. Mannodi-Kanakkithodi**, G. Pilania, T. Lookman, R. Ramprasad, "Machine Learning Bandgaps of Double Perovskites for Water-Splitting Applications", Symposium AAA: Big Data and Data Analytics for Materials Characterization, *Materials Research Society Fall Meeting*, Boston, Massachusetts, November 30 (2015).
- 2015 9. Oral: H.D. Tran, **A. Mannodi Kanakkithodi**, R. Ramprasad, "Accelerated materials property predictions and design using motif-based fingerprints", Section: Data and Tools for Materials Discovery and Design: Discovery and Design Infrastructure, *Materials Science and Technology (MS&T15)*, Columbus, Ohio, October 5 (2015).

- 2015 8. Oral: H.D. Tran, **A. Mannodi Kanakkithodi**, R. Ramprasad, "Accelerated materials property predictions and design using motif-based fingerprints", Section: From Chemical Data to Knowledge, *Gordon Research Seminar in Computer Aided Drug Design ? From Big Data to Smart Data*, West Dover, Vermont, July 19 (2015).
- 2014 7. Oral: **A. Mannodi-Kanakkithodi**, H.D. Tran, R. Ramprasad, "Organic Polymer Dielectrics Search via First Principles Computations and Machine Learning?", Symposium SS: Informatics and Genomics for Materials Development, *Materials Research Society Fall Meeting*, Boston, Massachusetts, December 2 (2014). *Best Student Oral Presentation Award*
- 2014 6. Oral: H.D. Tran, **A. Mannodi-Kanakkithodi**, C.C. Wang, R. Ramprasad, "Designing Organotin Polymers For Energy Storage Applications?", Symposium SS: Informatics and Genomics for Materials Development, *Materials Research Society Fall Meeting*, Boston, Massachusetts, December 1 (2014).
- 2014 5. Poster: H.D. Tran, **A. Mannodi-Kanakkithodi**, G. Pilania, R. Ramprasad, "Tin-based inorganic-organic hybrid polymers for high energy-density applications", Session P1: Poster Session III (DPOLY, DCP, DBIO, GSNP), *American Physical Society March Meeting*, Denver, Colorado, March 5 (2014).
- 2014 4. Poster: H.D. Tran, **A. Mannodi-Kanakkithodi**, C.C. Wang, A.F. Baldwin, R. Ma, G. Sotzing, R. Ramprasad, "Organotin polymeric dielectrics for energy-storage applications", Session P1: Poster Session III (DPOLY, DCP, DBIO, GSNP), *American Physical Society March Meeting*, Denver, Colorado, March 5 (2014).
- 2014 3. Oral: H.D. Tran, **A. Mannodi-Kanakkithodi**, C.C. Wang, A.F. Baldwin, R. Ma, G. Sotzing, R. Ramprasad, "First-principles design of organo-Sn polymeric dielectrics", Session B31: Computational Discovery and Design of New Materials II, *American Physical Society March Meeting*, Denver, Colorado, March 3 (2014).
- 2013 2. Poster: **A. Mannodi-Kanakkithodi**, C.C. Wang, R. Ramprasad, "Dielectric Permittivity Enhancement in Functionalized Polyolefins?", Symposium A: Modeling and Theory-Driven Design of Soft Materials, *Materials Research Society Fall Meeting*, Boston, Massachusetts, December 5 (2013).
- 2013 1. Poster: C. C. Wang, V. Sharma, **A. Mannodi-Kanakkithodi**, V. Botu, R. Ramprasad, "Comprehensive Examination of Dopants in BaTiO₃: From First Principles and Machine Learning?", Symposium NN: Strategies and Techniques to Accelerate Inorganic Materials Innovation, *Materials Research Society Fall Meeting*, Boston, Massachusetts, December 3 (2013). *Best Poster Award Nominee*

Upcoming Presentations

- 2019 1. Invited Tutorial: **A. Mannodi-Kanakkithodi**, "Machine Learning in Materials Informatics", *Introduction to Machine Learning for Solid State Chemistry: A Practical Workshop*, Colorado School of Mines, Golden, Colorado, July 29 (2019).

References

Prof. Rampi Ramprasad

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