COMPUTING & MATERIALS FRONTIERS

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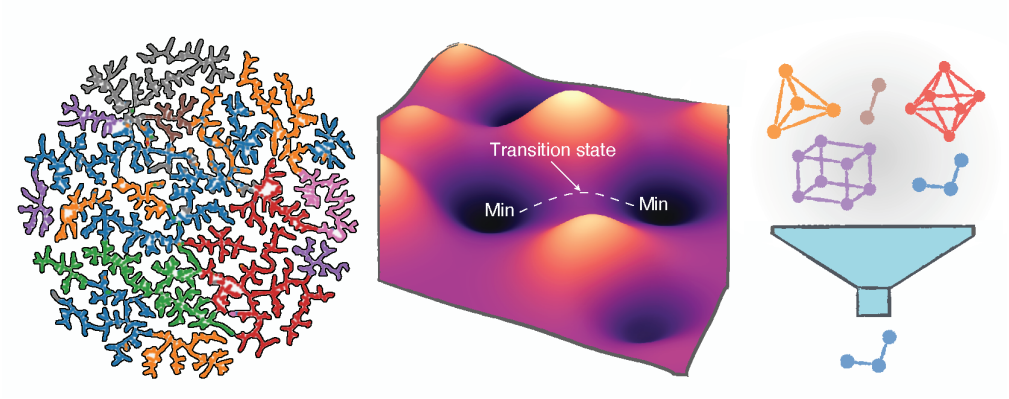
Dr. Wen is a Fellow of the Presidential Frontier Faculty program that supports faculty conducting highly interdisciplinary research. He obtained his Ph.D. from the University of Minnesota and was awarded the Doctoral Dissertation Fellowship for his work on the OpenKIM Project that strives to make molecular simulations reliable, reproducible and accessible. His postdoctoral work at Lawrence Berkeley National Laboratory focuses on the Materials Project, the world's leading materials genome project. Dr. Wen's expertise lies at the intersection of Materials Science, Chemical Engineering, and Computer Science. His research group specializes in leveraging data-driven methods such as artificial intelligence, high-performance computing, and atomistic molecular simulations to understand and design new molecules and materials for energy and electrochemical applications.

DATA-DRIVEN MATERIALS DISCOVERY



Machine Learning Reactions **Atomistic Molecular Simulation** **Materials Screening**

The overarching theme in Dr Wen's research is to design new data-driven computational approaches that can enable the investigation and discovery of materials in a more efficient and economical way. Insights from the computational study are used to inform experimental synthesis, characterization, and property design of novel materials.

Selected research topics in Dr. Wen's group include machine learning for chemical reactions, accelerated atomistic molecular simulations, and high-throughput computational matierals screening. His group has recently designed machine learning models that are able to represent any chemical reactions, as well as approaches to train such models with only a small amount of data. These models make it possible to do fast and accurate prediction of bond dissociation energies, reaction energies, and reaction types for the exploration of the gigantic chemical reaction space. They have also developed machine learning interatomic potentials to model the interactions between atoms and used them to perform large-scale atomistic molecular simulations to investigate lithium-ion batteries and nanoporous materials for energy storage and conversion. Another research area is designing high-throughput computational recipes based on density function theory to search for materials with exceptional mechanical and catalytic properties.

Publications

1. M Wen, EWC Spotte-Smit, SM Blau, MJ McDermott, AS Krishnapriyan, KA Persson, "Chemical reaction networks and opportunities for machine learning," Nature Computational Science, 3, 13-24, 2023. .

2. M Wen, SM Blau, X Xie, S Dwaraknath, and KA Persson, "Improving machine learning performance on small chemical reaction data with unsupervised contrastive pretraining," Chemical Science, 13, 1446-1458 (2022).

3. Z Shui, DS Karls, M Wen, IA Nikiforov, EB Tadmor, and G Karypis, "Knowledge distillation from empirical interatomic potentials to graph neural networks," 36th Conference on Neural Information Processing Systems (NeurIPS), 2022.

4. M Wen, Y Afshar, RS Elliott, and EB Tadmor, "KLIFF: A framework to develop physics-based and machine learning interatomic potential," Computer Physics Communication, 108218 (2021).

5. M Wen, SM Blau, EWC Spotte-Smith, S Dwaraknath, and KA Persson, "BonDNet: a graph neural network for the prediction of bond dissociation energies for charged molecules," Chemical Science, 12, 1858-1868 (2021).

6. M Wen and EB Tadmor, "Uncertainty quantification in molecular simulations with dropout neural network potentials," npj Computational Materials, 6, 124 (2020).

7. M Wen and EB Tadmor, "Hybrid neural network potential for multilayer graphene," Physical Review B, 100, 195419 (2019).

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