

Database for Harnessing Machine Learning to Advance Energy Materials



Nong Artrith

Debye Institute for Nanomaterials Science
Faculty of Science, Utrecht University, NL
Email: n.artrith@uu.nl



Dutch Sector Plan Project

May 19th, 2026
ChemSpider Webinar: Data Storage and Management

Publishing
Journals, books and databases

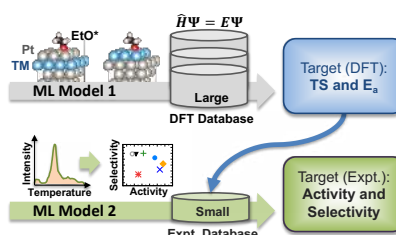


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Computational Discovery of Energy Materials and Interpretation of Experimental Observations with Atomistic First-Principles Methods and Machine Learning

Research Activities

Nong Artrith and Team
Computational Materials Science
and Machine Learning (ML)

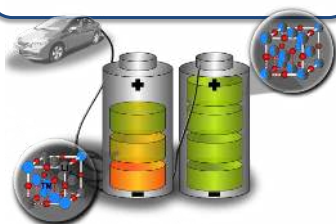


1. Machine Learning & Data Science

- Data from simulation and experiment (with collaborators)
- Accelerating DFT calculations
- Predicting materials properties
- Data mining for materials discovery

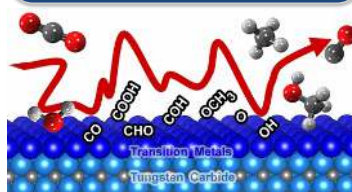
2. Energy Storage

- Storage for renewable energy
- Enable electric vehicles
- Improve portable electronics



3. Energy Conversion

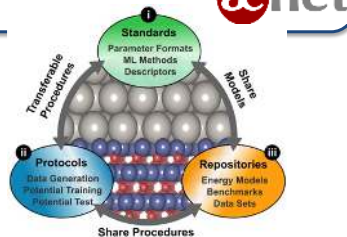
- Replace fossil fuels (oil/gas)
- Produce synthetic fuels using renewable energy



4. Method Development

- Open-source ML modeling tools

<https://github.com/atomisticnet>

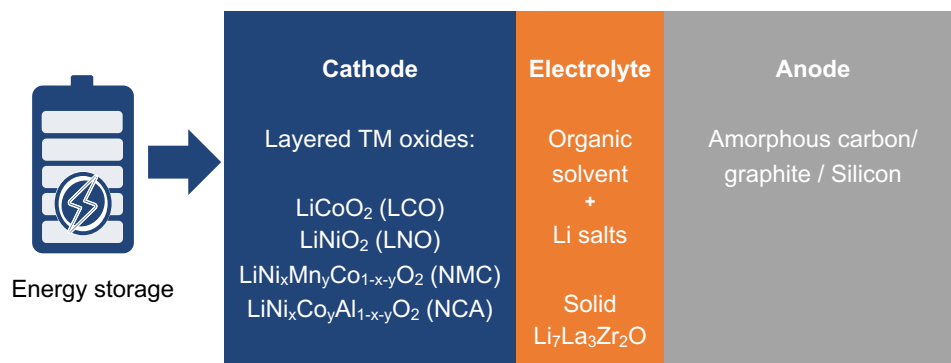


2

Batteries are Complex: Challenging for Simulation

- Elucidate the formation and structural evolution of interphases at solid-solid interfaces and the impact on the cell performance, to address the need for

“scientifically rational development of complex electrochemical interfaces”.



Movie source: US DOE

Nong Artrith (Email: n.artrith@uu.nl)

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Next-Generation Battery Materials



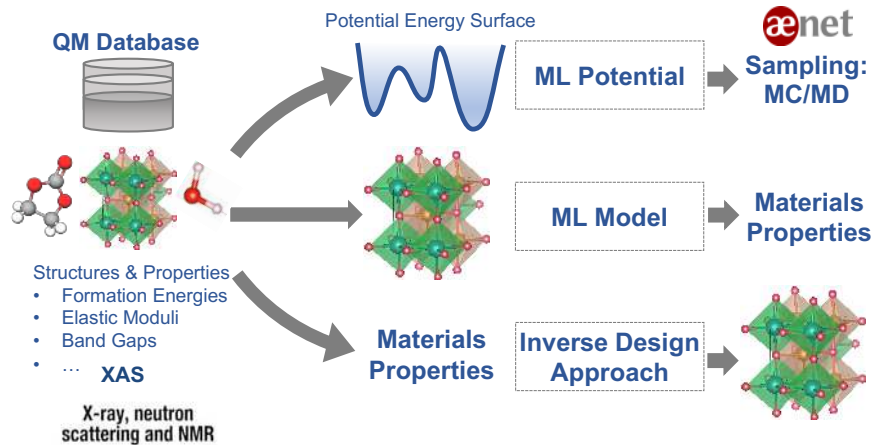
- [1] D. Bresser, K. Hosoi, D. Howell, H. Li, H. Zeisel, K. Amine, S. Passerini, *J. Power Sources* **382** (2018) 176-178.
 [2] <https://www.battery.nl>

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Machine Learning (ML) for Accelerated Modeling

- ML can be used to accelerate atomic-scale simulations
- ML models can also be trained on measured data to predict materials
- ML is also useful for the interpretation of measurements (e.g., from spectroscopy)

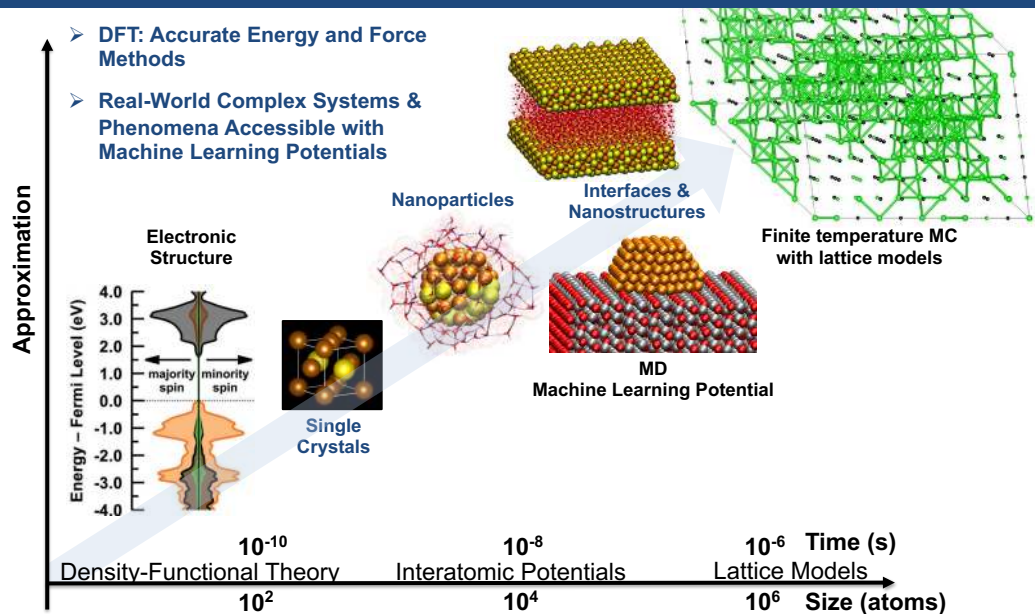


H. Guo, Q. Wang, A. Stuke, A. Urban, and **N. Artrith**, *Frontiers in Energy Research* 9, 2021, 695902

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Accurate Simulation of Large-Scale Systems

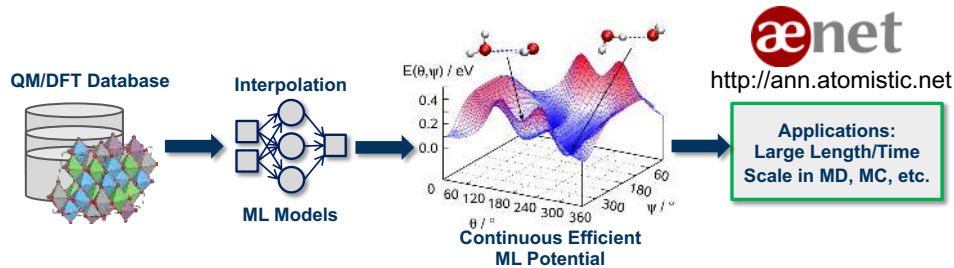


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Machine Learning Potentials for Complex Materials

- Learn from electronic structure theory (DFT) how atoms interact



• Our Approach:

- Artificial neural networks for interpolation
- Only based on atomic positions

⇒ As accurate as DFT
 ⇒ Reactive
 ⇒ + Full-dimensional

J. Behler, and M. Parrinello, *Phys. Rev. Lett.* 98, (2007) 146401.
 N. Artrith, T. Morawietz, and J. Behler, *Phys. Rev. B* 83, (2011) 153101.
 N. Artrith* and A. Urban, *Comput. Mater. Sci.* 114, (2016) 135-150.
 AM. Cooper, J. Kästner, A. Urban, and N. Artrith*, *npj Comput. Mater.* 6, (2020) 54.
 M.S. Chen, T. Morawietz, H. Mori, T.M. Markland, and N. Artrith*, *J. Chem. Phys.* 155, (2021) 074801
 T. Morawietz and N. Artrith*, *J. Comput. Aided. Mol. Des.* 35, (2021) 557.

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The ænet Package

The Atomic Energy Network



<http://ann.atomistic.net>

Alex Urban

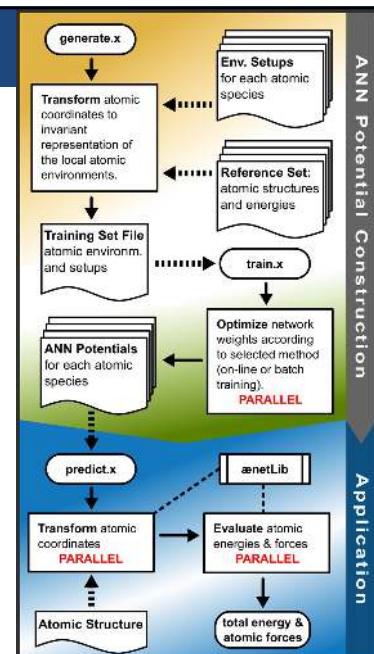


Jon Lopez

Modules for potential fit and for application

- C compatible library & Python interface
- MC/MD codes: ASE, LAMMPS, Tinker, DL_POLY, Genetic Algorithms

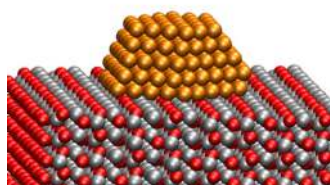
N. Artrith* and A. Urban, *Comput. Mater. Sci.* 114 (2016) 135-150.
 M.S. Chen, T. Morawietz, H. Mori, T.M. Markland, N. Artrith*, ænet-Lammps, *J. Chem. Phys.* 155 (2021) 074801.
 Jon Lopez-Zorrilla*, N. Artrith* et al, ænet-PyTorch, *J. Chem. Phys.* 158 (2023) 164105.



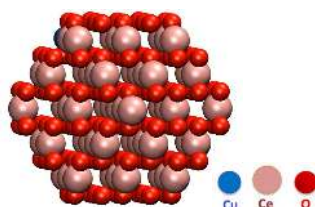
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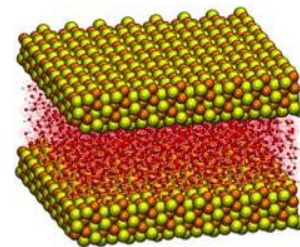
Accurate and Efficient ML: Non-Crystalline Nanostructures & Interphases



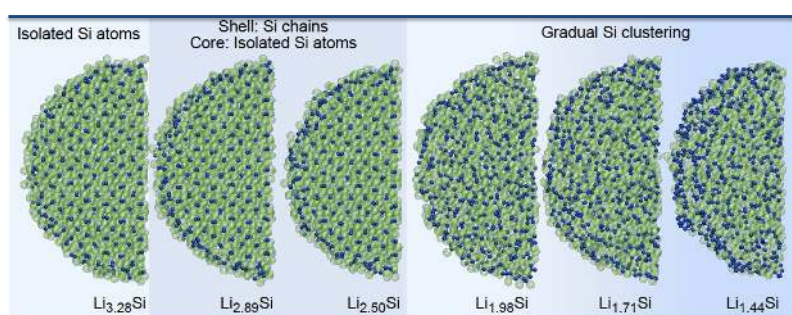
Cu/ZnO: [Artrith](#), Hiller, Behler, *Phys. Stat. Sol. B* 250 (2013) 1191.



CuO/CeO₂: Elias, [Artrith](#), Shao-Horn, et al., *ACS Catalysis* 6, (2016), 1675.



CuAu/H₂O: [Artrith](#)* and A.M. Kolpak, *Nano Lett.*, 14 (2014), 2670.



[Artrith](#)*, Urban, Ceder, *J. Chem. Phys.* 148, (2018) 241711 (Editor's Pick) and [arXiv:1901.09272 \(2019\)](#).

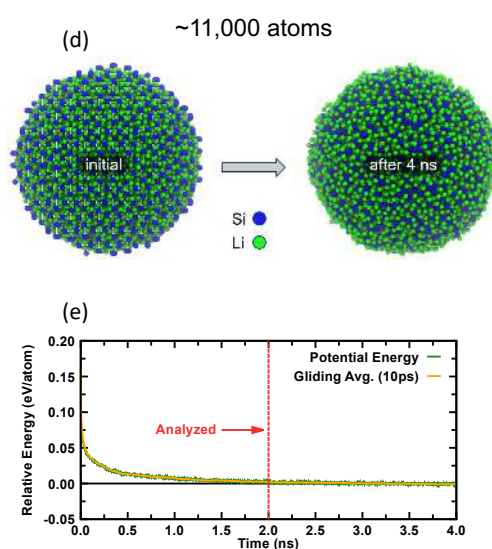
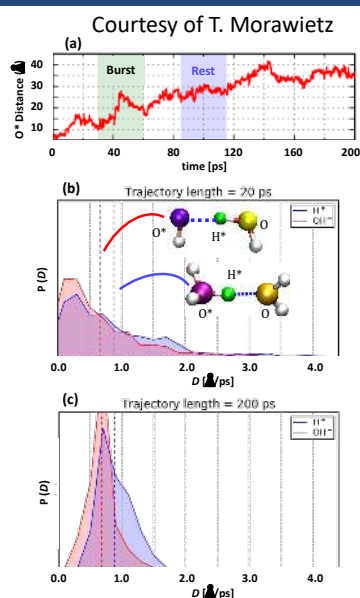
Lopez, [Artrith](#)* et al., [ænet-PyTorch](#): GPU support, *J. Chem. Phys.* 158 (2023) 164105.


http://ann.atomistic.net

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AENET-LAMMPS, AENET-TINKER



M.S. Chen, T. Morawietz, H. Mori, T.M. Markland, [N. Artrith](#)*, ænet-Lammps, ænet-Tinker: *JCP* (2021)

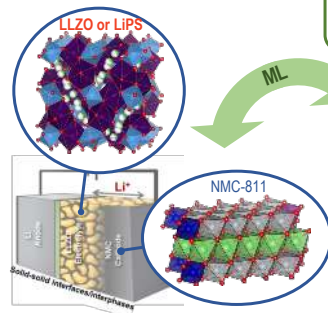
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Approach

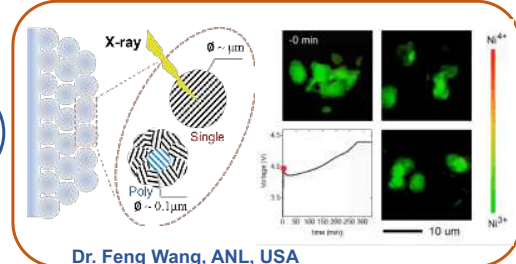
- **Challenge:** The interfacial degradation in solid-state battery cells involves phenomena on *multiple length* and *time scales*. Experimental characterization and first-principles modeling are disconnected.
- **Approach:** ML enabled by high-performance computing (HPC) to accelerate modeling and connect to experimental length and time scales.

State-of-the-art, ML-augmented
first-principles modeling



Bridging the gap between theory and experiment:
Structure-property relationships from
ML structural fingerprints and simulated spectroscopy

Cutting-edge *in situ* microspectroscopy



Dr. Feng Wang, ANL, USA

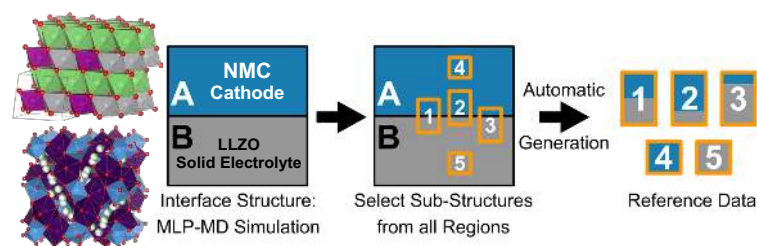
Feng Wang (ANL), Deyu Lu, Shinjae Yoo (BNL), Alex Urban (Columbia University), Nong Artrith (Utrecht University, NL)
Chuntian Cao and Matthew Carbone (BNL)

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Characterizing Interface Structures

Example: Motif (structural fingerprint) extraction in our ongoing solid-state battery interface project.



N. Artrith, *J. Phys. Energy* 1 (2019) 032002.

Our aim in the ongoing project: validate the computational $\text{Li}(\text{Ni}_x\text{Mn}_y\text{Co}_z)\text{O}_2$ (NMC)/ $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) or LiPS models by comparison with spectroscopy

Collaboration: more general **database** that can be reused in future projects for automatic interpretation of X-ray spectra of interface systems

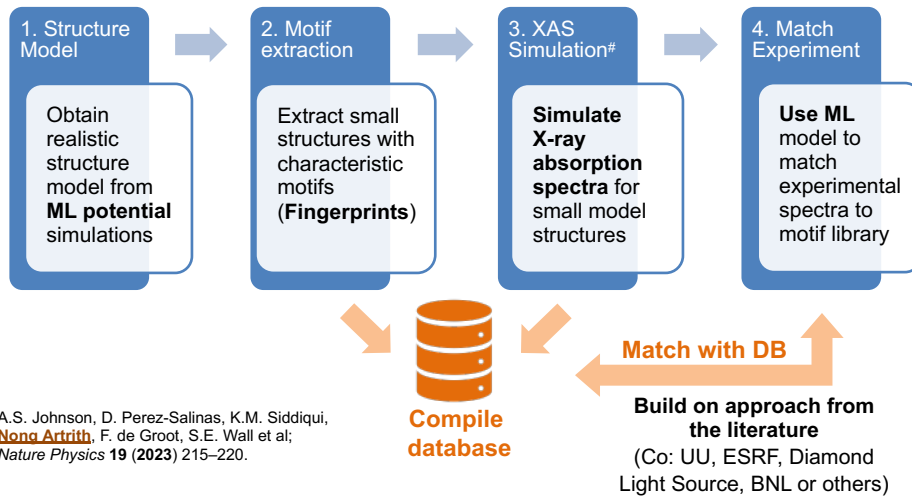
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Characterization of Interface Structures

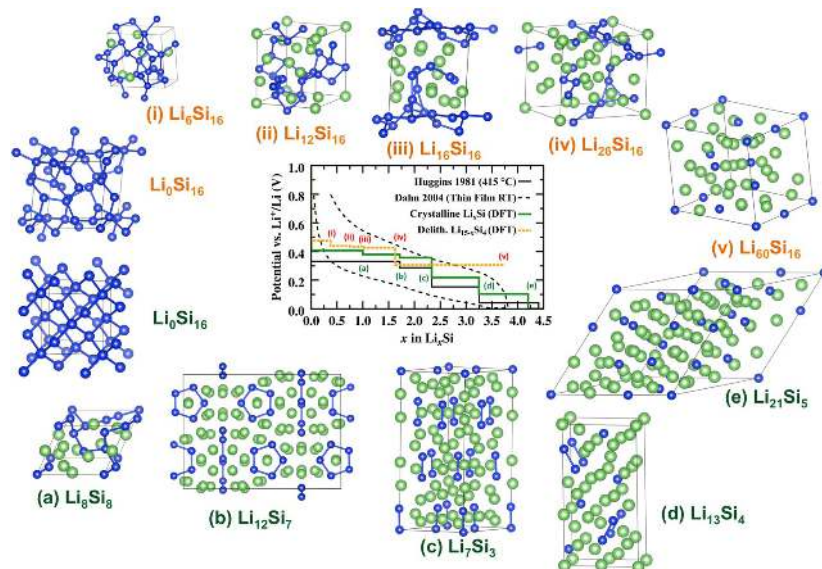
- Machine learning (ML) for the automated interpretation of X-ray absorption spectra from interface systems with e.g., transition-metal oxides



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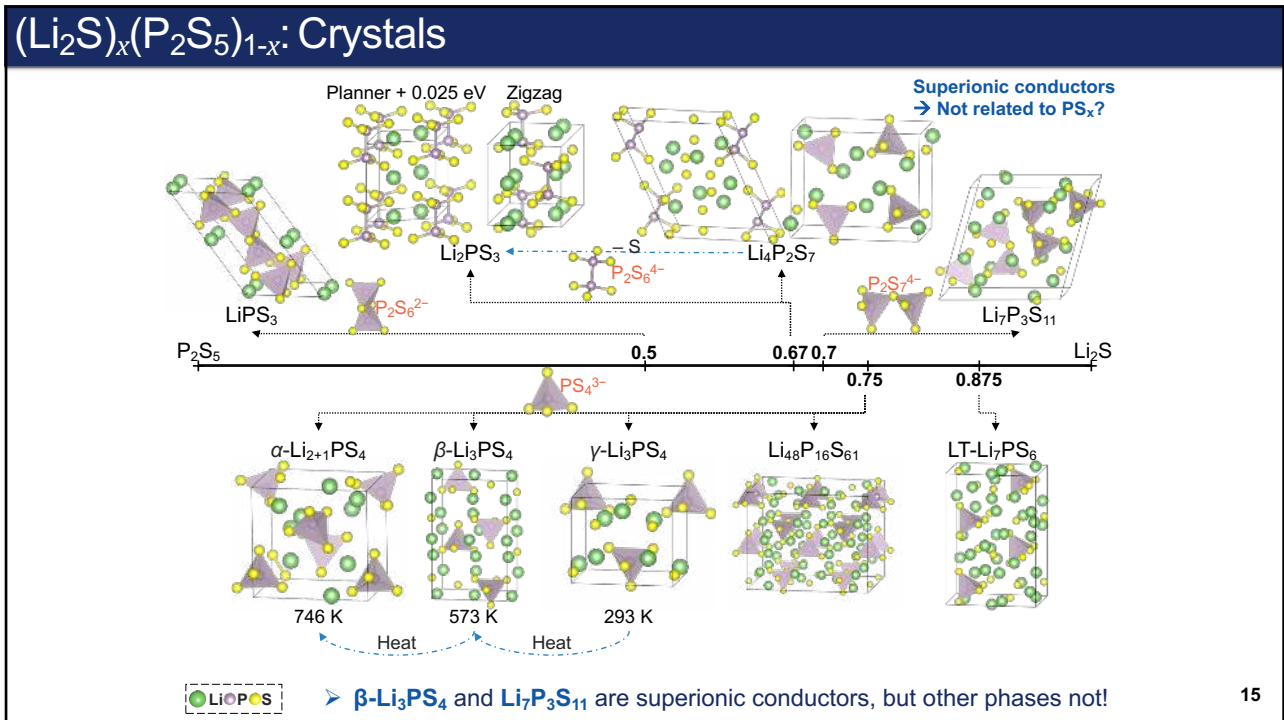
(x in Li_xSi): Phase Diagram



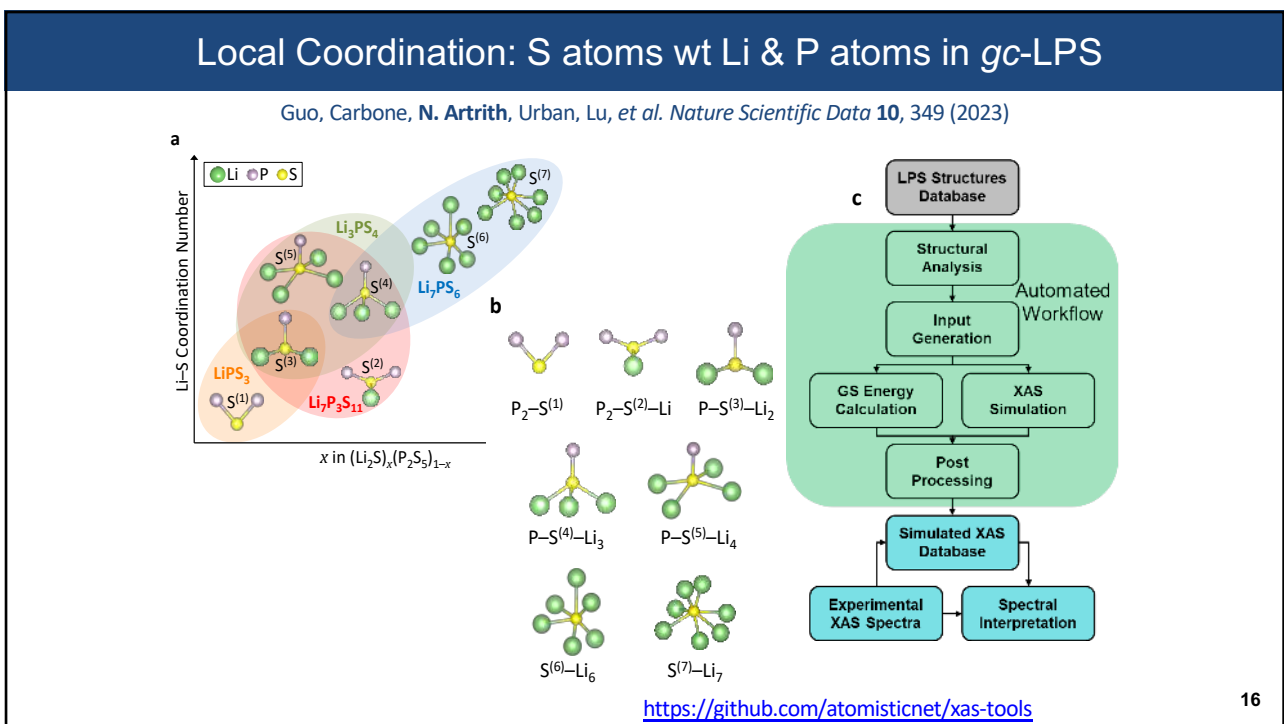
M.S. Chen, T. Morawietz, H. Mori, T.M. Markland, **N. Artrith**^{*}, ænet-Lammps, ænet-Tinker: *JCP* (2021)
 Jon Lopez-Zorrilla^{*}, **N. Artrith**^{*} et al, ænet-PyTorch: a GPU-supported: *JCP* (2023)

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Structure database of glass-ceramic lithium thiophosphate electrolytes

DOI: [10.24435/materialscloud.js-7z](https://doi.org/10.24435/materialscloud.js-7z) v1

Guo, Haoyue; Artrith, Nongnuch

This database contains computationally generated atomic structures of glass-ceramics lithium thiophosphates (gc-LPS) with the general composition $(\text{Li}_2\text{S})_x(\text{P}_2\text{S}_5)_{1-x}$ in the XCrySDen structure format (XSF). Total energies and interatomic forces from density-functional theory (DFT) calculations are included as additional meta information. The extends...

Latest version: v1

Publication date: February 1, 2022

1065 153

Efficient Training of ANN Potentials by Including Atomic Forces via Taylor Expansion and Application to Water and a Transition-Metal Oxide

DOI: [10.24435/materialscloud:2020.0837v1](https://doi.org/10.24435/materialscloud:2020.0837v1) v1

Cooper, April; Kästner, Johannes; Urban, Alexander; and 1 other

This data set contains atomic structures of water clusters, bulk water and rock-salt $\text{Li}_8\text{Mo}_2\text{Ni}_7\text{Ti}_7\text{O}_{32}$ in the XCrySDen [1] structure format (XSF), and total energies are included as additional meta information. The extended XSF format is compatible with the atomic energy network (aenet) package [2,3] for artificial neural network potential constru...

Latest version: v1

Publication date: April 14, 2020

633 216

N. Artrith (n.artrith@uu.nl): <https://github.com/atomisticnet>

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materialscloud:2023.59

Published April 12, 2023 | Version v3 Dataset Open

Simulated sulfur K-edge X-ray absorption spectroscopy database of lithium thiophosphate solid electrolytes

Guo, Haoyue^{1,*}; Carbone, Matthew R.^{2,*}; Cao, Chuntian²; Qu, Jianzhou¹; Wang, Feng^{3,4}; Yoo, Shinjae²; Artrith, Nongnuch^{1,5,6,*}; Urban, Alexander^{1,5,7,*}; Lu, Dayu^{8,*}

* Contact person

Show affiliations

We present a sulfur K-edge X-ray absorption near-edge structure (XANES) database of 18 crystalline and 48 amorphous Lithium-Phosphorous-Sulfur (LPS) compounds. The database contains a total of 2681 XANES spectra of symmetrically inequivalent absorbing S sites. Structures were taken from Materials Cloud entry 2022.17 (archive.materialscloud.org/record/2022.17) and were originally generated by systematically removing Li, P and S atoms from known crystal structures using an evolutionary algorithm and an artificial neural network based interatomic potential. The details of this procedure can be found in Guo et al. (see references below). From this data set, low-energy structures were selected for spectral simulations. The excited electron and core hole method as implemented in VASP 6.2.1 was used to compute the XANES spectra for each symmetrically inequivalent Sulfur atom. The details of the VASP simulations can be found in the associated manuscript. Acknowledgements: We acknowledge financial support by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Office, Contract No. DE-SC0012704. These results used the computational resources of the Center for Functional Nanomaterials and the Scientific Data and Computing Center, a component of the Computational Science Initiative, at Brookhaven National Laboratory under the Contract No. DE-SC0012704. We also acknowledge computing resources from Columbia University's Shared Research Computing Facility project, which is supported by NIH Research Facility Improvement Grant 1G20RR030693-01, and associated funds from the New York State Empire State Development, Division of Science Technology and Innovation (NYSTAR) Contract C090171, both awarded April 15, 2010.

N. Artrith (n.artrith@uu.nl): <https://github.com/atomisticnet>

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atomistic.net

54 followers <http://ann.atomistic.net>

Popular repositories

- aenet** (Public) - Atomic interaction potentials based on artificial neural networks. Fortran, 128 stars, 44 forks.
- tools-and-data** (Public) - A collection of tools and databases for atomistic machine learning. 48 stars, 10 forks.
- MLP-beginners-guide** (Public) - Strategies for the Construction of Neural-Network Based Machine-Learning Potentials (MLPs). Jupyter Notebook, 29 stars, 9 forks.
- mi-catalysis** (Public) - Machine Learning for Catalysis. Jupyter Notebook, 20 stars, 11 forks.
- xas-tools** (Public) - Tools related to X-ray absorption spectroscopy (XAS). Python, 19 stars, 4 forks.
- aenet-PyTorch** (Public) - aenet-PyTorch: a GPU-supported implementation for machine learning atomic potentials training. Fortran, 17 stars, 5 forks.

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CatMine-LLM Private

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CatMine-LLM

LLM-Enabled Literature Mining Workflow for Cu-Based CO₂ Hydrogenation Catalysts Development

Overview

CatMine-LLM is an open, reproducible workflow that applies large language models (LLMs) to mine and structure unstructured scientific literature on copper-based CO₂ hydrogenation catalysts. The project introduces a standardized catalytic profile schema that links catalyst descriptors, reaction conditions, performance metrics, and

About

CatMine-LLM: LLM-Enabled Literature Mining Workflow for Cu-Based CO₂ Hydrogenation Catalysts Development

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N. Artrith (n.artrith@uu.nl): <https://github.com/atomisticnet>

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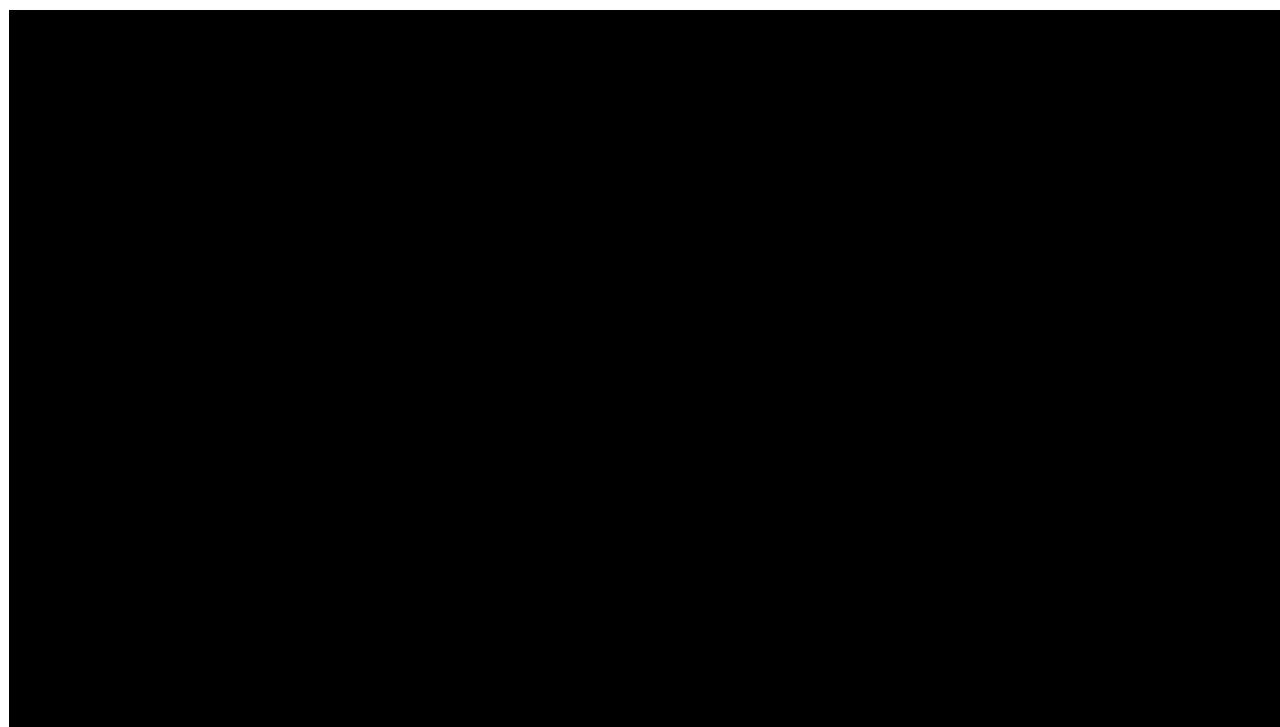
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