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EDUCATION

Materials Science and Engineering, Ford-Northwestern University Alliance, Evanston, IL, The U.S.
Aug. 2023 – Present
Postdoctoral Fellow in Materials Science | **PI:** Prof. Chris Wolverton
Major research: Data-Driven Search for Novel Li-Rich Layered Oxides (LRLO) Battery Chemistries; Machine Learning (ML)-Based Design and Discovery of Li-ion Battery Materials and Complex Nanoparticles

Materials Science and Engineering, National University of Singapore (NUS), Singapore
Aug. 2019 – Jul. 2023
Ph.D. in Materials Science and Engineering; CAP: 4.75/5.0
Major Project: Optimization and Discovery of Positive Electrode Materials Beyond Lithium-Ion Batteries with First-Principles Multiscale Techniques | **Supervisor:** Asst. Prof. Pieremanuele Canepa

School of Physics, University of Chinese Academy of Sciences (UCAS), Beijing, P. R. China
Sept. 2015 - Jul. 2019
Bachelor of Science in Physics; Overall GPA: 3.75/4.0; Major GPA: 3.8/4.0 (top 5% in the department)
Final Year Project: Mechanics of Growth of Two-Dimensional Au_2Se Atomic Crystal Thin Film Material | **Advisor:** Prof. Xiao Lin & Hongjun Gao

RESEARCH INTERESTS

- Design and simulation for energy storage, and applications, including electrode/electrolyte materials for Na/Li-ion batteries, all-solid-state batteries, thin film materials, nanoparticles, and semiconductors
- Combine high-throughput computations with techniques from statistical mechanics modelling & ML to facilitate investigations of novel energy materials
- Multiscale methods combining theoretical computations and experimental characterizations to understand fundamental physics of properties of materials

RESEARCH EXPERIENCES

Postdoc Fellow, Ford-Northwestern Alliance **Aug. 2023 – Present**
PI: Prof. Chris Wolverton

- **Overview:** Combine high-throughput computations and ML models to design novel LRLO (i.e., Li- and Mn-rich (LMR) layered oxides) battery cathode, with improved electrochemical properties and industrial cost; significantly extend current materials database (e.g., to include materials interfacial properties) and develop ML tools for accelerating exploration of new materials.
- **Project 1:** Using multi-compositional substitution strategies to stabilize the structure of LMR (i.e., Li_2MnO_3) at high-voltage region with constrained cation migration and oxygen release, assisted by high-throughput computations || Understand phase behaviours of Li_2MnO_3-$LiMO_2$ compounds (M = Ni, Mn, Co)[1] || Construct ML-database for key properties of LRLO cathodes (e.g., $LiMO_2$-Li_2MO_3 composites) in large chemical space, with self-developed models & packages.

- **Project 2:** Data-driven design and discovery of complex nanoparticles with controlled interfacial properties.
- **Project 3:** Computationally-assisted investigations of novel perovskites.

Ph.D. Graduate Research Assistant, NUS **Aug. 2019 – Jul. 2023**
Supervisor: Asst. Prof. Pieremanuele Canepa

- **Overview:** Combined first-principles calculations with statistical mechanics analysis (i.e., cluster expansion, Monte Carlo simulation) and ML tools for multiscale discovery and optimization of electrode/electrolyte materials for Na-ion batteries.
  - In cooperation with **TIAMAT Energy** / Laboratoire de Réactivité et de Chimie des Solides (**LRCS**) / Université de Picardie Jules Verne (**UPJV**) / **CNRS**-UMR / **RS2E** / University of California, San Barbara (**UCSB)** / Indian Institute of Science (**IISc**) / Bar Ilan University (**BIU**) / University of Houston (**UH**)
- **Project 1:** Investigated thermodynamic properties and Na (de)intercalation mechanisms of NaSICON electrodes through a *3d*-transition metal based chemical space. (B. Singh, **Z. Wang** et al. ***J. Mater. Chem. A***[2])
- **Project 2:** Elucidated complex thermodynamics of Na intercalation into NaSICON-based $Na_xV_2(PO_4)_3$ cathode combining first-principles calculations, cluster expansion, and Monte Carlo simulations. Identified a new stable phase of $Na_2V_2(PO_4)_3$ using computations and experiments. (**Z. Wang**, S. Park et al. ***J. Mater. Chem. A***[3]***, Chem. Mater.***[4] & **Patent** WO-2023209113-A1)
- **Project 3:** Developed a novel chemical synthesis method to obtain various unconventional stable phases of $Na_xV_2(PO_4)_3$ (e.g., $Na_{1.75}V_2(PO_4)_3$, $Na_2V_2(PO_4)_3$, $Na_{2.25}V_2(PO_4)_3$) and reached $V_2(PO_4)_3$ by complete Na-extraction from single-phase $Na_xV_2(PO_4)_3$ cathode. Increased the theoretical energy density to 458 Wh/kg at an average voltage of 3.7 V vs. Na/Na^+. (S. Park, **Z. Wang** et al. ***Nature Materials***[5])
- **Project 4:** Developed a python-based kinetic Monte Carlo simulation package to capture the effect of local configuration on Na-ion transport in NaSICON electrodes**. (Z. Wang** et al. ***ACS Materials Lett.***[6]**)**
- **Project 5:** Optimized energy density of $Na_xV_2(PO_4)_2F_3$ electrode by unlocking its inaccessible capacities at high-voltage region through transition metal/anion mixing. (S. C. C. van der Lubbe, **Z. Wang** et al. ***Chem. Mater.***[7]**,** S. Chakrabarty et al.)
- **Project 6:** Developing cluster expansion model for "liquid-like" lattices.

Undergraduate Thesis, UCAS **Nov. 2018 – May 2019**
Advisor: Prof. Xiao Lin & Hongjun Gao

- **Overview:** Utilized chemical vapor deposition for generating two-dimensional Au_2Se crystal thin film material. Unveiled mechanics of growth of the as-synthesized material and investigated its surface topology combining atomic force microscope, X-ray photoelectron spectroscopy and X-ray diffraction.

Undergraduate Research Assistant, UCLA **Jul. 2018 – Aug. 2018**
Advisor: Prof. Gerard C. L. Wong

- **Overview:** Experiments on high-speed "4D" computational microscopy of bacterial surface motility.

Undergraduate Research Assistant, Institute of Physics, CAS **Dec. 2017 – Apr. 2018**
Advisor: Prof. Xiao Lin, Hongliang Lu

- **Overview:** Mechanical exfoliation and surface morphology characterisation of 2D materials.

PUBLICATIONS

Published:

- 1. *Phase Stability of Li-Rich Layered Cathodes: Insight into the Debate over Solid Solutions vs Phase Separation.* Z. Lu, S. Hao, **Z. Wang**, H. Kim, C. Wolverton, ***Chem. Mater.*** **2024**, acs.chemmater.2c00927.

- 2. *A Chemical Map of NaSICON Electrode Materials for Sodium-Ion Batteries.* B. Singh¶, **Z. Wang¶**, S. Park, G. S. Gautam, J.-N. Chotard, L. Croguennec, D. Carlier, A. K. Cheetham, C. Masquelier, P. Canepa, ***J. Mater. Chem. A - Themed Collections: HOT Papers; Energy Frontiers; Battery science and technology*** **2021**, *9* (1), 281–292. **¶Equal Contribution**
- 3. *Phase Stability and Sodium-Vacancy Orderings in a NaSICON Electrode.* **Z. Wang**, S. Park, Z. Deng, D. Carlier, J.-N. Chotard, L. Croguennec, G. S. Gautam, A. K. Cheetham, C. Masquelier, P. Canepa, ***J. Mater. Chem. A - Themed Collection: HOT Papers*** **2022**, *10* (1), 209–217.
- 4. *Crystal Structure of $Na_2V_2(PO_4)_3$, an Intriguing Phase Spotted in the $Na_3V_2(PO_4)_3$ –$Na_1V_2(PO_4)_3$ System*. S. Park, **Z. Wang**, Z. Deng, I. Moog, P. Canepa, F. Fauth, D. Carlier, L. Croguennec, C. Masquelier, J.-N. Chotard, ***Chem. Mater.*** **2022**, *34* (1), 451–462.
- 5. *Obtaining $V_2(PO_4)_3$ by Sodium Extraction from Single-Phase $Na_xV_2(PO_4)_3$ ($1 < x < 3$) Positive Electrode Materials.* S. Park¶, **Z. Wang¶**, K. Choudhary, J.-N. Chotard, D. Carlier, F. Fauth, P. Canepa, L. Croguennec, C. Masquelier, ***Nature Materials.*** **2024**. **¶Equal Contribution**
- 6. *Kinetic Monte Carlo Simulations of Sodium Ion Transport in NaSICON Electrodes.* **Z. Wang**, T. P. Mishra, W. Xie, Z. Deng, G. S. Gautam, A. K. Cheetham, P. Canepa, ***ACS Materials Lett.*** **2023,** *5*(9), 2499-2507
- 7. *Unlocking the Inaccessible Energy Density of Sodium Vanadium Fluorophosphate Electrode Materials by Transition Metal Mixing.* S. C. C. Van Der Lubbe¶, **Z. Wang¶**, D. K. J. Lee, P. Canepa, ***Chem. Mater.*** **2023**, *35* (13), 5116–5126. **¶Equal Contribution**

In-Progress (Selected):

- *Effect of Nb Substitution on Thermodynamic and Kinetic Properties of $Na_xV_2(PO_4)_3$*. E. G. Correa, **Z. Wang**, F. Zhou, P. Canepa, R. Clément.
- *Impact of Br Substituted $Na_3V_2(PO_4)_2F_{(3-x)}Br_x$ Structure Towards Triggering of 3rd Na During Reversible Na (de)Intercalation for Na Ion Battery*. S. Chakrabarty, A. Mukherjee, **Z. Wang**, S. Taragin, R. Yemini, I. Perelshtein, P. Canepa, M. Noked.
- *Sodium-Vacancy and Vanadium-Manganese Orderings in Mn-Substituted $Na_xV_2(PO_4)_3$ NaSICON Cathode.* **Z. Wang**, M. Bhatt, P. Canepa.
- *Advanced CASM Package with Accuracy in "Liquid-Like" Crystal Lattices.* **Z. Wang**, P. Canepa.
- *A Machine-Learning Approach for Screening Key Properties of Lithium-Rich Layered Oxides.* **Z. Wang**, C. Wolverton.
- *Optimization of Ion-Exchange Lithium-Rich and Mn-Rich Layered Oxides with Multi-Compositional Defects.* **Z. Wang**, Y. Han, C. Liu, C. Wolverton.
- *An Isomeric Homologous Series of Perovskite in Ba-Sb-Te-S Chemical Space.* H. Zhao, **Z. Wang**, S. Shahabfar, S. Hao, C. Wolverton, M. Kanatzidis.
- *Structural Stabilization of A Layered Manganese Oxide with Reversible Oxygen Redox at High Voltage.* Z. Liu, **Z. Wang**, C. Wolverton, Q. Liu.
- *Investigation into Charge Transition by Ionic Migrations for Anion Redox in Layered Oxides.* Z. Liu, **Z. Wang**, C. Wolverton, Q. Liu, Y. Ren.

PATENT

- *New Nasicon-Type High Voltage Sodium Vanadium Phosphates Materials For Na-Ion Batteries*. S. Park, J.-N. Chothard, L. Croguennec, D. Carlier-Larregaray, C. Masquelier, **Z. Wang** and P. Canepa, WO-2023209113-A1.

CONFERENCES

- 2021 The Electrochemical Society (ECS) Meeting Abstract. *Crystal Chemistry of $Na_xMM'(PO_4)_3$ Nasicon Electrodes (M, M' = V, Fe, Mn, Ti, Cr)*.
- 2022 The 2nd International Conference on Materials for Humanity (MRS-MH 22) Poster Presenter. *Sodium-vacancy Orderings and Crystal Structures of $Na_xV_2(PO_4)_3$ NaSICON Electrodes.*

- 2023 The International Conference on Materials for Advanced Technologies (ICMAT) Meeting Abstract. *New Vanadium Phosphates as Positive Electrode Materials for Na-ion and K-ion Batteries.*
- 2024 International Meeting on Lithium Batteries (IMLB) Poster Presenter. *Investigation and Optimization of Li-Rich Layered Oxide Cathodes with High-Throughput Computations and Beyond.*
- 2024 The Solid State Chemistry Gordon Research Conference (GRC) Poster Presenter. *Linking Sodium Solubility to Ion Transport in Natrium Super Ionic CONductors.*

TEACHING EXPERIENCES

- **Teaching Assistant:** Module MLE 3101 @ NUS **2020 Semester #2 & 2021 Semester #2**
  Organized and mentored laboratory-based lectures. Assisted students with hands-on thin-film materials characterization using atomic force microscopy.
- **Research Assistant:** Canepa Research Group @ NUS **2019 - 2023**
  Assisted with research group activities, including periodical group meeting organizations, compute clusters management, junior students mentorship, and research outreach & collaboration arrangement.

HONORS & AWARDS

- Undergraduate Academic Scholarship | Oct. 2018
- Yuan Hong (Shan Dong) Technical Materials Ltd's Public Scholarship | Apr. 2018
- NUS Research Scholarship | Aug. 2019 – Jul. 2023
- Ford-Northwestern Alliance Postdoctoral Fellowship | Aug. 2023 – Present
- Northwestern the International Institute for Nanotechnology Future Faculty Program 2024 Participant

SKILLS

- **Experimental skills**: Thermal evaporation / Mechanical exfoliation / Atomic Force Microscopy (AFM) / X-ray Diffraction (XRD) / X-ray photoelectron spectroscopy (XPS) / Nuclear magnetic resonance (NMR)
- **Programming skills**: Windows/Linux system, C, C++, Python, ML, Shell
- **Softwares**: Microsoft Office, VASP, CASM, Lobster, ATAT, QuantumEspresso, CASTEP, VESTA