# Jun Meng

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## Professional Preparation

Shanghai Institute of Applied Physics, CAS, China — 2014 – 2019
*Ph.D. Materials Science, Supervisor: Prof. Yi Gao*

University of Science and Technology of China — 2014 – 2015
*Visiting student*

Henan Normal University, China — 2010 – 2014
*B.S., Physics*

## Appointments

University of Wisconsin-Madison, USA — 2020 – present
*Research Associate, Advisor: Prof. Dane Morgan*

Institute Charles Gerhardt Montpellier, CNRS, France — 2018 – 2019
*Research Assistant, Advisor: Prof. Hazar Guesmi*

## Research Interest & Accomplishments

**Research interest:**
I apply theory and first-principles methods to understand and explore the structure and properties of materials critical for clean energy applications, including fuel cells, solid-state batteries, and solar cells. My focus is on ion transport in solid-state systems, interfaces, and metastable phases, utilizing advanced atomic-scale modeling, multiscale simulation, materials informatics methods, and data-driven machine learning approaches.

**Selected accomplishments:**

- Developed the first method for discovering new interstitial oxygen diffusers, identified multiple new families and validated $La_4Mn_5Si_4O_{22}$ as a novel superior oxygen conductor. This research has resulted in two first author papers and one patent.
- Developed the StructOpt algorithm which integrates experimental data with real-time atomic simulations to optimize the realistic atomic structure that capturing both short- and medium-range ordering characteristics of amorphous materials, enhancing structure-property understanding and targeted materials design. This work has yielded one first author paper, five contributed papers, and one patent.
- Developed the first theoretical model, Multiscale Structure Reconstruction (MSR), which accurately simulates the dynamic shape evolution of nanoparticles catalysts under varying reactive environment, including temperature, pressure, surroundings, and supports, enhancing in-situ performance evaluations and catalyst design. This research has resulted in four first author papers, six co-first author papers, and five contributed papers.

## Software Tools

- Lead developer on Multiscale Operando Simulation Package (MOSP: www.mosp.top), designed to reproduce and visualize the equilibrium geometries of nanoparticles under reaction conditions with selectable size, temperature, pressure, surroundings, and supports.
- Lead developer on Structure determination of amorphous oxides guided by multiple inputs from experiments and simulations. (https://github.com/uw-cmg/StructOpt/tree/TiO2)

## Patents

1. Dane D. Morgan, Ryan M. Jacobs, and **Jun Meng**. *Oxygen Ion Transport Materials and Related Devices* (filed on June 15, 2021 by Wisconsin Alumni Research Foundation (WARF), *in processing*)
2. Xudong Wang, Yutao Dong, Dane Morgan, **Jun Meng**, Jinwoo Hwang, Mehrdad Abbasi Gharacheh. *Substantial Lifetime Enhancement of Si-Based Photoanodes Enabled by Amorphous $TiO_2$ Coating with Improved Stoichiometry* (filed on July 17, 2023 by Wisconsin Alumni Research Foundation (WARF), *in processing*)

## Publications **(13 first-author, 8 second-author, 7 co-author, 1 *in submission* first-author, Google Scholar H-index: 12, citation > 500)**

1. **J. Meng**, Md. S. Sheikh, R. Jacobs, J. Liu, W. O. Nachlas, X. Li and D. Morgan, Ultra-fast Oxygen Conduction in Sillén Oxychlorides. ***In submission***, Arxiv.org/abs/2406.07723v1.
2. **J. Meng**, Md. S. Sheikh, R. Jacobs, J. Liu, W. O. Nachlas, X. Li and D. Morgan, Computational Discovery of Fast Interstitial Oxygen Conductors. ***Nat. Mater.* 2024,** DOI: 10.1038/s41563-024-01919-8.
3. X. Li, P. Ou, X. Duan, L. Ying**, J. Meng,** B. Zhu, and Y. Gao, Dynamic Active Sites In Situ Formed in Metal Nanoparticle Reshaping under Reaction Conditions. ***JACS Au* 2024,** 4 (5), 1892-1900.
4. Y. Dong, M. Abbasi, **J. Meng,** L. German, C. Carlos, J. Li, Z. Zhang, D. Morgan, J. Hwang, X. Wang. Substantial lifetime enhancement for Si-based photoanodes enabled by amorphous $TiO_2$ coating with improved stoichiometry. ***Nat. Commun.* 2023,** 14, 1865.
5. M. Abbasi, **J. Meng,** Y. Dong, D. Morgan, X. Wang, and J. Hwang, EELS / 4D-STEM Investigation of Development of Local Atomic Orderings within ALD-grown Amorphous $TiO_2$ Films, ***Microscopy and Microanalysis* 2023,** 29 (S1), 405–406.
6. M. Abbasi, Y. Dong, **J. Meng,** D. Morgan, X. Wang, J. Hwang, *In situ* observation of medium range ordering and crystallization of amorphous $TiO_2$ ultrathin films grown by atomic layer deposition. ***APL Mater.* 2023,** 11 (1): 011102. (**Editor's pick & Journal Cover**)
7. **J. Meng,** M. Abbasi, Y. Dong, C. Carlos, X. Wang, J. Hwang, D. Morgan, Experimentally informed structure optimization of amorphous TiO2 films grown by atomic layer deposition. ***Nanoscale* 2023,** 15, 718–729.
8. M. Abbasi, **J. Meng,** Y. Dong, D. Morgan, X. Wang, and J. Hwang, In-Situ 4D-STEM Study of Amorphous Titanium Oxide for Water Splitting Application, ***Microscopy and Microanalysis* 2022,** 28 (S1), 442–443.
9. P. Yu, **J. Meng,** *et al.* Carbonate-Ion-Mediated Photogenerated Hole Transfer to Boost Hydrogen Production. ***J. Phys. Chem. C* 2022,** 126 (25), 10367–10377
10. B. Wu, X. Zhan, P. Yu, **J. Meng,** *et al.* Photocatalytic co-production of hydrogen gas and N-benzylidenebenzylamine over high-quality 2D layered In4/3P2Se6 nanosheets. ***Nanoscale* 2022,** 14, 15442-15450.
11. **J. Meng,** B. Zhu, Y. Gao, Structure Reconstruction of Metal/Alloy in Reaction Conditions: A Volcano Curve? ***Faraday Discuss.* 2021**, 229, 62–74.
12. M. Abbasi, **J. Meng,** Y. Dong, D. Morgan, X. Wang, and J. Hwang, 4D-STEM Determination of Atomic Structure of Amorphous Materials for Renewable Energy Applications, ***Microscopy and Microanalysis* 2021,** 27 (S1), 396–398.
13. P. Yu, F. Wang, **J. Meng,** T. Shifa, M. Sendeku, J. Fang, S. Li, Z. Cheng, X. Lou and J. He, Few-layered CuInP2S6 nanosheet with sulfur vacancy boosting photocatalytic hydrogen evolution. ***CrystEngComm* 2021,** 23, 591-598
14. B. Zhu, **J. Meng (co-first author),** W. Yuan, X. Zhang, H. Yang, Y. Wang, Y. Gao, Reshaping of Metal Nanoparticles in Reaction Conditions. ***Angew. Chem. Int. Ed.* 2020**, 59, 2171–2180.
15. S. Song, **J. Meng,** Y. Wang, J. Zhou, L. Zhang, N. Gao, C. Guan, G. Xiao, Z. Hu, H.-J. Lin, C.-T. Chen, X.-L. Du, J. Hu, J.-Q Wang, Molten Salt Treated Cu Foam Catalyst for

Selective Electrochemical CO2 Reduction Reaction. ***ChemistrySelect*** **2020**, 5, 11927.

16. A. Khelfa, **J. Meng,** C. Byun, G. Wang, J. Nelayah, C. Ricolleau, H. Amara, H. Guesmi and D. Alloyeau, Selective shortening of gold nanorods: when surface functionalization dictates the reactivity of nanostructures. ***Nanoscale*** **2020,** 12, 22658-22667.
17. D. Alloyeau, A. Khelfa, K. Aliyah, A. Chmielewski, **J. Meng,** H. Amara, H. Guesmi, J. Nelayah, G. Wang, C. Hamon, D. Constantin, C. Ricolleau, Revealing the Dynamics of Functional Nanomaterials in Their Formation and Application Media with Liquid and Gas-phase TEM. ***Microscopy and Microanalysis*** **2020,** 26 (S2), 196–198.
18. **J. Meng**, B. Zhu, Y. Gao. Surface Composition Evolution of Bimetallic Alloys under Reaction Conditions. ***J. Phys. Chem. C*** **2019**, 123 (46), 28241–28247.
19. **J. Meng**, C. Hou, H. Wang, Q. Chi, Y. Gao, B. Zhu, Water-Driven Oriented Attachment Growth of Monocrystalline Cuprous Oxide Nanowires: Novel Experimental Observation and Rational Understanding. ***Nanoscale Adv.*** **2019**, 2174-2179. (**Journal Cover**)
20. A. Chmielewski, **J. Meng** (**co-first author**), *et al.*, Reshaping Dynamics of Gold Nanoparticles under $H_2$ and $O_2$ at Atmospheric Pressure. ***ACS Nano***, **2019**, *13*, 2024-2033.
21. J. Du, **J. Meng,** X-Y Li, B. Zhu and Y. Gao, Multiscale atomistic simulation of metal nanoparticles under working conditions. ***Nanoscale Adv.*** **2019**, 1, 2478-2484.
22. M. Duan, J. Yu, **J. Meng,** B. Zhu, Y. Wang, Y. Gao, Reconstruction of Supported Metal Nanoparticles in Reaction Conditions. ***Angew. Chem. Int. Ed.*** **2018**, 130 (22), 6574–6579.
23. **J. Meng**, B. Zhu, Y. Gao, Shape Evolution of Metal Nanoparticles in Binary Gas Environment. ***J. Phys. Chem. C*** **2018**, *122*, 6144-6150.
24. W. Yuan, **J. Meng** (**co-first author**), B. Zhu, Y. Gao, Z. Zhang, C. Sun, Y. Wang, Unveiling the atomic structures of the minority surfaces of $TiO_2$ nanocrystal, ***Chem. Mater.*** **2018**, *30*, 288-295.
25. X. Zhang, **J. Meng** (**co-first author**), B. Zhu, W. Yuan, H. Yang, Z. Zhang, Y. Gao and Y. Wang, *Chem. Commun.*, Unexpected refacetting of palladium nanoparticles under atmospheric $N_2$ conditions. ***Chem. Commun.*** **2018**, *54*, 8587-8590.
26. M. Tang, B. Zhu, **J. Meng,** X. Zhang, W. Yuan, Z. Zhang, Y. Gao, Y. Wang. Pd–Pt nanoalloy transformation pathways at the atomic scale. ***Materials Today Nano*** **2018,** 1, 41-47.
27. X. Zhang, **J. Meng** (**co-first author**), B. Zhu, J. Yu, S. Zou, Z. Zhang, Y. Gao, Y. Wang, In situ TEM studies of Shape Evolution of Pd Nanocrystals under Oxygen and Hydrogen Environment at Atmospheric Pressure, ***Chem. Commun.*** **2017**, *53*, 13213-13216.
28. B. Zhu, **J. Meng** (**co-first author**), Y. Gao, Equilibrium Shape of Metal Nanoparticles under Reactive Gas Conditions, ***J. Phys. Chem. C*** **2017**, *121*, 5629-5634.

## Presentations (1 invited, 9 contributed)

1. New Family of Interstitial Oxygen Ion Conductor Discovered By High-Throughput Computational Screening. **Poster**, 243rd ECS Meeting with the 18th International Symposium on Solid Oxide Fuel Cells (SOFC-XVIII), Boston, USA, 2023
2. Discovery of New Fast Oxygen Conductors: $Bi_2MO_4X$ (M= rare earth, X= halogen) Via Unsupervised Machine Learning. **Poster**, 243rd ECS Meeting with the 18th International Symposium on Solid Oxide Fuel Cells (SOFC-XVIII), Boston, USA, 2023
3. New Family of Interstitial Oxygen Ion Conductor Discovered by High-Throughput Computational Screening. **Oral talk.** TMS2023, San Diego, USA. 2023
4. New Fast Oxygen Ion Conductor Perrierite-Type Oxide $La_4Mn_5Si_4O_{22+\delta}$ Discovered by Harnessing the Materials Project and High-Throughput Computation. **Oral talk.** 2022 MRS Fall Meeting, Boston, USA. 2022
5. Experimentally Informed Structure Optimization of Amorphous $TiO_2$ Films Grown by Atomic Layer Deposition. **Poster**, 2022 MRS Fall Meeting, Boston, USA. 2022 (**Best Poster Award**)
6. Multiscale Simulation of Reshaping of Metal Nanoparticles in Reaction Conditions. **Invited talk,** Theoretical Computation of Solids and Surfaces "Young Scholars" Forum, Zhejiang, China. 2019
7. Multiscale Structure Reconstruction (MSR) Model for Predicting the Shape Evolution of

Metallic Nanoparticles under Reaction Conditions: from Monometallic to Nanoalloy. **Oral talk**, GDR NanOperando, Lyon, France. 2018

8. Multiscale Structure Reconstruction (MSR) Model for Predicting the Shape Evolution of Metallic Nanoparticles under Reaction Conditions: from Monometallic to Nanoalloy. **Oral talk**. International Meeting on Nanoalloys, Orlean, France. 2018
9. Multiscale Structure Reconstruction (MSR) Model for Predicting the Shape Evolution of Au Nanoparticles under Reaction Conditions. **Poster**, Au-Nano, Montpellier, France. 2018
10. Equilibrium Shape of Metal Nanoparticles under Reactive Gas Conditions. **Poster**, The 14th National Conference on Quantum Chemistry of the Chinese Chemical Society. Dalian, China 2017

## Awards

- Best Poster Award. MRS Fall Meeting 2022
- Outstanding Doctoral Graduates. Chinese Academy of Sciences 2020
- Postgraduate National Scholarship. Chinese Academy of Sciences 2019
- Outstanding Student. Chinese Academy of Sciences 2019

## Skills

**Simulation & computer skills**

- First-principles calculations
- Molecular dynamics
- Monte carol simulations
- Multi-scale modeling
- High-throughput computing
- Materials datamining
- Machine learning potential
- VASP, LAMMPS, Gaussian
- Python

**Laboratory Skills**

- Solid-state synthesis
- X-ray diffraction analysis
- UV-Vis Spectroscopy
- 4-Probe conductivity measurements
- Electrical Conductivity Relaxation (ECR)

## Synergistic Activities

- Volunteer at the University of Wisconsin-Madison Engineering Expo, which seeks to engage and educate K-12 children and the public in a wide range of scientific principles.
- Judge at Wisconsin Capital Science & Engineering Fair, which provides high school students the opportunity to showcase their research at a national competition.

## Reviewer for peer-reviewed journals

Journal of physical chemistry, Nano Trends, IEEE Transactions on Electron Devices, Physica status solidi., Sensors and actuators.