

Jun Meng, PhD

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Professional Preparation

Ph.D. Materials Science , Shanghai Institute of Applied Physics, CAS, China	2020
<i>Thesis: Theoretical Study of the Structure of Metal Nanoparticle under Real Reaction Conditions.</i>	
Joint Ph.D. candidate , Institute Charles Gerhardt Montpellier, CNRS, France	2019
Joint Ph.D. candidate , University of Science and Technology of China	2015
B.S. Physics , Henan Normal University, China	2014

Appointments

Postdoc Research Associate , University of Wisconsin-Madison, USA	2020 – present
Research Assistant , Institute Charles Gerhardt Montpellier, CNRS, France	2018 – 2019
Research Assistant , Shanghai Institute of Applied Physics, CAS, China	2015 – 2020

Research Interest & Accomplishments

My research focuses on using theory and first-principles methods to explore materials critical for clean energy, such as fuel cells, solid-state batteries, and solar cells. I specialize in ion transport in solid-state systems, interfaces, and metastable phases, employing atomic-scale modeling, multiscale simulations, materials informatics, machine learning, and experiments. Below are selected main accomplishments:

2020-Now

- Developed the materials informatic approach of discovering new fast oxygen conductors, identified multiple new families and experimentally validated $\text{La}_4\text{Mn}_5\text{Si}_4\text{O}_{22+d}$ as a novel superior oxygen conductor. (2 papers, 1 patent)
- Developed the StructOpt algorithm which integrates multiple inputs from both experiments and simulations to optimize the realistic atomic structure for meta-stable phases, enabling structure-property understanding for amorphous materials. (6 papers, 1 patent, 1 code).

2015-2020

- Developed the first theoretical model, Multiscale Structure Reconstruction (MSR), to reproduce the shape evolution of nanoparticles under real reaction, due to the changing temperature, pressure, surroundings, and supports. (15 papers, 1 code)

Publications (12 first-author, 9 second-author, 7 co-author, [Google Scholar](#) citation > 550)

2024

- J. Meng**, Md. S. Sheikh, L. Shultz, W. O. Nachlas, J. Liu, M. Polak, R. Jacobs, and D. Morgan, Ultra-fast Oxygen Conduction in Sillén Oxychlorides. *In revision*, [Arxiv.org/abs/2406.07723v1](https://arxiv.org/abs/2406.07723v1).
- 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.
- X. Zheng, **J. Meng**, N. Guisinger, J. Guest, K. Su, D. Morgan, M. Arnold, Evolution of PTCDA-derived seeds prior to graphene nanoribbon growth on Ge(001). *Carbon* 2024, 229, 119468.
- 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.

2023

- J. Meng**, M. Abbasi, Y. Dong, C. Carlos, X. Wang, J. Hwang, D. Morgan, Experimentally informed structure optimization of amorphous TiO_2 films grown by atomic layer deposition. *Nanoscale* 2023, 15, 718–729.
- 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.

7. 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 TiO₂ Films, *Microscopy and Microanalysis* 2023, 29 (S1), 405–406.
8. M. Abbasi, Y. Dong, **J. Meng**, D. Morgan, X. Wang, J. Hwang, *In situ* observation of medium range ordering and crystallization of amorphous TiO₂ ultrathin films grown by atomic layer deposition. *APL Mater.* 2023, 11 (1): 011102. (Editor's pick & Journal Cover)

2022

9. 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.
10. 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
11. 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.

2021

12. **J. Meng**, B. Zhu, Y. Gao, Structure Reconstruction of Metal/Alloy in Reaction Conditions: A Volcano Curve? *Faraday Discuss.* 2021, 229, 62–74.
13. 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.
14. P. Yu, F. Wang, **J. Meng**, T. Shifa, M. Sendeku, J. Fang, S. Li, Z. Cheng, X. Lou and J. He, Few-layered CuInP₂Se₆ nanosheet with sulfur vacancy boosting photocatalytic hydrogen evolution. *CrystEngComm* 2021, 23, 591–598

2020

15. 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.
16. 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.
17. A. Khelifa, **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.
18. D. Alloyeau, A. Khelifa, 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.

2019

19. **J. Meng**, B. Zhu, Y. Gao. Surface Composition Evolution of Bimetallic Alloys under Reaction Conditions. *J. Phys. Chem. C* 2019, 123 (46), 28241–28247.
20. **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)
21. A. Chmielewski, **J. Meng (co-first author)**, *et al.*, Reshaping Dynamics of Gold Nanoparticles under H₂ and O₂ at Atmospheric Pressure. *ACS Nano*, 2019, 13, 2024–2033.
22. 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.

2018

23. 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 TiO₂ nanocrystal, *Chem. Mater.* 2018, 30, 288-295.

24. 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 N₂ conditions. *Chem. Commun.* 2018, 54, 8587-8590.
25. 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.
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.

2017

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.

Patents

- Dane D. Morgan, **Jun Meng**, and Ryan M. Jacobs. *Oxygen Ion Transport Materials and Related Devices*. US Patent App. 18/565,772, 2024
- Xudong Wang, Yutao Dong, Dane Morgan, **Jun Meng**, Jinwoo Hwang, Mehrdad Abbasi Gharacheh. *Substantial Lifetime Enhancement of Si-Based Photoanodes Enabled by Amorphous TiO₂ Coating with Improved Stoichiometry* (filed on July 17, 2023, in processing)

Software/Tool Developed

- 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>)

Presentations (2 invited, 13 contributed)

Oral talks. ECS PRiME. Hawai'i, USA	upcoming
Poster , Gordon Research Conference - Solid State Studies in Ceramics. MA, USA	2024
Posters , 243rd ECS Meeting, SOFC-XVIII. Boston, USA	2023
Oral talk. TMS2023. San Diego, USA	2023
Oral talk & Poster. MRS Fall Meeting (Best Poster Award). Boston, USA	2022
Invited Oral talk. International Forum on Advanced Materials. Peking University, China	2022
Poster , DOE PI's meeting	2020
Invited Oral talk. Theoretical Computation of Solids and Surfaces, Zhejiang University, China	2019
Oral talk , GDR NanOperando, Lyon, France.	2018
Oral talk. International Meeting on Nanoalloys, Orlean, France.	2018
Poster , Au-Nano, Montpellier, France.	2018
Poster , National Conference on Quantum Chemistry. Dalian, China	2017

Grant /Fellowship/Awards

Grant

Advanced computing and data resource program. U.S. National Science Foundation, Award # MAT240071	2024
ECS Travel Grant (\$1,000), PRiME	2024

Fellowship

National Scholarship (\$4,500), Chinese Academy of Sciences	2019
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China – France “Cai Yuanpei” Program Fellowship (\$20,000), China National Science Foundation 2017

Awards

Finalist for the 5th Rising Stars Award in Computational Materials Science 2024

Best Poster Award (\$300), MRS Fall Meeting 2022

Outstanding Ph.D. Graduate of the Year Award, Chinese Academy of Sciences 2020

Outstanding Ph.D. Student Award (\$150), Chinese Academy of Sciences 2019

Skills

Simulation & computer skills		Laboratory Skills
• First-principles calculations	• Machine learning potential	• Solid-state synthesis
• Molecular dynamics	• Materials datamining	• X-ray diffraction analysis
• Multi-scale modeling	• VASP, LAMMPS, Gaussian	• UV-Vis Spectroscopy
• High-throughput computing	• Python	• 4-Probe conductivity measurements
• Monte carol simulations		• Electrical Conductivity Relaxation (ECR)

Academic Services

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- **Discussion leader** at 2024 Solid State Studies in Ceramics, Gordon Research Seminar.
 - **Reviewer** for peer-reviewed journals: Journal of physical chemistry, Nano Trends, IEEE Transactions on Electron Devices, Physica status solidi., Sensors and actuators.
 - **Volunteer** for scientific outreach: Wisconsin Capital Science & Engineering Fair; University of Wisconsin-Madison Engineering Expo.