Jun Meng, PhD

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Professional Preparation

Ph.D. Materials Science, Shanghai Institute of Applied Physics, CAS, China 2020
Thesis: Theoretical Study of the Structure of Metal Nanoparticle under Real Reaction Conditions.
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 $La_4Mn_5Si_4O_{22+d}$ 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 software)

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

2024

1. **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.
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. 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.
4. 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

5. **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.
6. 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 TiO_2 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 TiO_2 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 CuInP2S6 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. 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.
18. 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.

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 H_2 and O_2 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 TiO_2 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 N_2 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 TiO_2 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

China – France "Cai Yuanpei" Program Fellowship ($20,000), China National Science Foundation 2017

Awards

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

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

Laboratory Skills

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

Academic Services

- **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.