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Research

Emergent Materials and Intelligent TEM (EMIT) Lab aims to advance the synthesis, characterization, and analysis of emergent functional materials via developing AI-driven combinational toolkit. Our research focuses on three interconnected areas:

1. Intelligent Synthesis: We develop automated robotic systems for high-throughput chemical synthesis and automated sample preparation for structural and functional characterization. Synthetic routes are dynamically optimized in real time based on AI-guided analysis of characterization data.
2. Intelligent Characterization: We develop intelligent transmission electron microscopy (TEM) techniques, including novel hardware for liquid-cell TEM and advanced data analysis algorithms for in situ and 4D TEM. These innovations enable us to uncover the fundamental structure-property relationships at the atomic scale.
3. Artificial Intelligence: We leverage AI techniques to design hierarchical materials, predict their structures and properties, and develop intelligent algorithms for analyzing complex characterization datasets, particularly from in situ and high-throughput experiments.

Representative Study Systems

- **High-Performance Ni-Based Catalysts for Seawater Electrolysis:** Combining robotic synthesis and Bayesian optimization algorithms to develop record-performing nickel-based catalysts for efficient seawater electrolysis.
- **AI-Driven Sensing Arrays for Drug and Biomarker Detection:** Designing ultra-sensitive sensing arrays with AI-powered data analysis to enhance the detection of drugs and biomarkers.
- **Advanced In Situ TEM for Electrochemical Systems:** Developing novel liquid-cell TEM techniques to achieve atomic-resolution imaging in electrochemical environments.
- **Automated Structural Recognition for TEM Data:** Creating AI-driven algorithms for automatic structural recognition in complex TEM datasets, enabling detailed insights into battery material interfaces.
- **Chemistry-Informed Neural Networks for Semiconductor Analysis:** Developing AI models informed by chemistry to analyze the structure-property relationships of semiconductors, supported by DFT calculations.

Work Experience

2021.08–	South China University of Technology, Professor
2017.08–2021.05	MSE, UC Berkeley, Postdoc MSD, Lawrence Berkeley National Laboratory, Postdoc
Supervisor:	Prof. Haimei Zheng
2016.05–2017.08	Department of Polymer Science, Akron University, Postdoc
Supervisor:	Prof. Stephen Z. D. Cheng

Education

2009.09–2016.05 Xiamen University, Department of Chemistry
Advisors: Prof. Zhong-qun Tian; Prof. Xiaoyu Cao

2005.09–2009.05 Nanjing University, Kuang Yaming Honors School
Advisor: Prof. Hong Yan

Teaching

1. Introduction to AI for Chemistry and Materials
2. Scientific writing and illustration

Publications

A graphic-enriched online version can be found on my website: Link.

[30] C. Chen, L. Cao, Y. Liu, Z. Li, Z. Li, G. Zhou, D. Zhang, X. Huang, Y. Wang*, G. Li, L. Liu, Y. Yuan, Y. Zhang, Q. Wang, Y. Chen, Z. Shi, Q. Fang, Z. Huang, Z. Lai, and Y. Han*. Investigating a Seemingly Simple Imine-Linked Covalent Organic Framework Structure.
J. Am. Chem. Soc., 2024, 10.1021/jacs.4c16678.

[29] Y. Meng, M. Wang, J. Wang, X. Huang, X. Zhou, M. Sajid, Z. Xie, R. Luo, Z. Zhu, Z. Zhang, N. Khan, Y. Wang*, Z. Li*, and W. Chen*. Robust bilayer solid electrolyte interphase for Zn electrode with high utilization and efficiency.
Nat. Commun., **2024**, 15, 8431.

[28] X. Liu, X. Yan*, Y. Liu, H. Qu, Y. Wang, J. Wang, Q. Guo, H. Lei, X. Li, F. Bian, X. Cao, R. Zhang, Y. Wang, M. Huang, Z. Lin, E. W. Meijer, T. Aida, X. Kong*, and S. Z.D. Cheng*. Self-assembled soft alloy with Frank–Kasper phases beyond metals.
Nat. Mater., **2024**, 23, 570.

[27] Y. Meng, M. Wang, K. Li, Z. Zhu, Z. Liu, T. Jiang, X. Zheng, K. Zhang, W. Wang, Q. Peng, Z. Xie, Y. Wang, and W. Chen*. Reversible, dendrite-free, high-capacity aluminum metal anode enabled by aluminophilic interface layer.
Nano Lett., **2023**, 23, 2295.

[26] Y. Xie, J. Wang, B. Savitzky, Z. Chen, Y. Wang, S. Betzler, K. Bustillo, K. Persson, Y. Cui, L. Wang, C. Ophus*, P. Ercius*, and H. Zheng*. Spatially resolved structural order in low-temperature liquid electrolyte.
Sci. Adv., **2023**, 9, eadc9721.

[25] Y. Wang,# Z. Song,# J. Wan, S. Betzler, Y. Xie, C. Ophus, K. Bustillo, P. Ercius, L. Wang, and H. Zheng*. Strong structural and electronic coupling in metavalent PbS moiré superlattices.
J. Am. Chem. Soc., **2022**, 144, 23474.

[24] Z. Song,# Y. Wang,# H. Zheng, P. Narang,* and L. Wang*. Deep quantum-dot arrays in moiré superlattices of non-van der Waals materials.
J. Am. Chem. Soc., **2022**, 144, 14657.

[23] Q. Zhang,# Z. Song,# Y. Wang,# Y. Nie, J. Wan, K. Bustillo, P. Ercius, L. Wang, L. Sun, and H. Zheng*. Swap motion–directed twinning of nanocrystals.
Sci. Adv., **2022**, 8, eabp9970.

[22] Y. Liu, Tong Liu, X. Yan, Q. Guo, H. Lei, Z. Huang, R. Zhang, **Y. Wang**, J. Wang, F. Liu, F. Bian, E.W. Meijer, T. Aida, M. Huang*, and Stephen Z.D. Cheng*. Expanding quasiperiodicity in soft matter: Supramolecular decagonal quasicrystals by binary giant molecule blends.
Proc. Natl. Acad. Sci. USA, **2022**, 119, e2115304119.

Prior to joining SCUT (2021.08)

[21] J. Jiang, **Y. Wang**, L. Jin, C-H Hsu, S. Zhang, J. Mao, W. Yin, T. Li, B. Ni, Z. Su, J. Huang, C. Wesdemiotis, K. Yue, W. Zhang*, and S. Z. D. Cheng*. Modularly constructed polyhedral oligomeric silsesquioxane-based giant molecules for unconventional nanostructure fabrication.
ACS Appl. Nano Mater., **2020**, 10.1021/acsanm.0c00231.

[20] **Y. Wang**,† X. Peng,† A. Abelson, P. Xiao, C. Qian, L. Yu, C. Ophus, P. Ercius, L-W. Wang, M. Law, and H. Zheng*. Dynamic deformability of individual PbSe nanocrystals during superlattice phase transitions.
Sci. Adv., **2019**, 5, eaaw5623 (†Equal contribution)
Highlighted by Molecular Foundry, Lawrence Berkeley National Lab.

[19] H. L. Zhang,† **Y. Wang**,† H. Zhang,† X. Liu,† A. Lee, Q. Huang, F. Wang J. Chao, H. Liu, J. Li, J. Shi, X. Zuo, L. Wang, L. Wang, X. Y. Cao, C. Bustamante, Z. Q. Tian*, and C. H. Fan*. Programming chain-growth co-polymerization of DNA hairpin tiles for in-vitro hierarchical supramolecular organization.
Nat. Commun., **2019**, 10, 1006 (†**Equal contribution**)

[18] **Y. Wang**,† Y. Sun,† P. Shi, X. Lin, P. Zhang, H. Fang, P. Peng, Z. Q. Tian, and X. Cao*. Chaperone-like chiral cages for catalyzing enantioselective supramolecular polymerization.
Chem. Sci., **2019**, 10, 8076 (†Equal contribution)
Selected as Front Cover, Editor's Pick of the Week, and 2019 Chemical Science HOT Article Collection. Highlighted by RSC news as "Coaching catalysis".

[17] **Y. Wang**, X. Peng, A. Abelson, B. Zhang, P. Ercius, L-W. Wang, M. Law, and H. Zheng*. Atomic-resolution in situ observation of the necking phenomenon during oriented attachment of PbSe nanocrystals
Nano Res., **2019**, 12, 2549

[16] Z. Su, C. Hsu, Z. Gong, X. Feng, J. Huang, R. Zhang, **Y. Wang**, J. Mao, C. Wesdemiotis, T. Li, S. Seifert, W. Zhang, T. Aida, M. Huang*, and S. Z.D. Cheng*. Identification of a Frank–Kasper Z phase from shape amphiphile self-assembly.
Nat. Chem., **2019**, 11, 899.

[15] R. Lu, X. Yan, L. Zhu, L. Yang, H. Qu, X. Wang, M. Luo, **Y. Wang**, R. Chen, X. Wang*, Y. Lan*, J. Pei, W. Weng, H. Xia, and X. Cao*. Unveiling how intramolecular stacking modes of covalently linked dimers dictate photoswitching properties.
Nat. Commun., **2019**, 10, 5480.

[14] Q. Zhang, G. Gao, Y. Shen, X. Peng, J. Shangguan, **Y. Wang**, H. Dong, K. Bustillo, L. Wang, L. Sun, and H. Zheng*. Anomalous shape evolution of Ag_2O_2 nanocrystals modulated by surface adsorbates during electron beam etching.
Nano Lett., **2019**, 19, 591.

[13] X. X. Peng, A. Abelson, **Y. Wang**, C. Qian, J. Shangguan, Q. Zhang, L. Yu, Z. W. Yin, W. Zheng, K. C. Bustillo, X. Guo, H. G. Liao*, S. G. Sun, M. Law, and H. M. Zheng*. In situ TEM study of the degradation of PbSe nanocrystals in air.
Chem. Mater., **2019**, 31, 190.

[12] **Y. Wang**,† H. X. Fang,† I. Tranca, H. Qu, X. C. Wang, A. J. Markvoort*, Z. Q. Tian, and X. Y. Cao*. Elucidation of the origin of chiral amplification in discrete molecular polyhedra.
Nat. Commun., **2018**, 9, 488 (†Equal contribution)

[11] Z. A. Nan, **Y. Wang***, Z. X. Chen, S. F. Yuan, Z. Q. Tian, and Q. M. Wang*. Catalyzed assembly of hollow silver-sulfide cluster through self-releasable anion template.
Commun. Chem. **2018**, 1, 99. (***Corresponding author**)

[10] X. C. Wang, P. X. Peng, W. Xuan, **Y. Wang**, Y. B. Zhuang, Z. Q. Tian, and X. C. Cao*. Narcissistic chiral self-sorting of molecular face-rotating polyhedra.
Org. Biomol. Chem., **2018**, 16, 34.

[9] H. Qu, **Y. Wang***, Z. H. Li, X. C. Wang, H. X. Fang, Z. Q. Tian, and X. Y. Cao*. Molecular face-rotating cube with emergent chiral and fluorescence properties.
J. Am. Chem. Soc., **2017**, 139, 18142. (***Corresponding author**) (**Cover paper**)

[8] **Y. Wang**, H. X. Fang, W. Zhang, Y. B. Zhuang, Z. Q. Tian, and X. Y. Cao*. Interconversion of molecular face-rotating polyhedra through turning inside out.
Chem. Commun., **2017**, 53, 8956 (**Cover paper**)

[7] **Y. Wang***, Y. B. Sun, X. B. Ding, J. H. Liang, X. Y. Cao, and Z. Q. Tian*. A combined electro- and photo-chemical approach to repeatedly fabricate 2D molecular assemblies.
Electrochim. Acta., **2017**, 246, 823. (***Corresponding author**)

[6] Z. W. Lin, J. Sun, Y.B. Zhou, **Y. Wang**, H. Xu, X. Yang, H. Su, H.G. Cui, T. Aida, W. Zhang*, and S. Z.D. Cheng*. A noncrystallization approach toward uniform thylakoids-like 2D "nano-coins" and their grana-like 3D suprastructures.
J. Am. Soc. Chem., **2017**, 139, 5883.

[5] X. C. Wang,† **Y. Wang**,† H. Y. Yang, H. X. Fang, R. X. Chen, Y. B. Sun, N. F. Zheng, K. Tan, X. Lu, Z. Q. Tian, and X. Y. Cao*. Assembled molecular face-rotating polyhedra to transfer chirality from two to three dimensions.
Nat. Commun., **2016**, 7, 12469. (†**Equal contribution**)

[4] L. Q. Xie, T. Y. Zhang, L. Chen, N. Guo, **Y. Wang**, G. K. Liu, J. R. Wang, J. Z. Zhou, J. W. Yan, Y. X. Zhao*, B. W. Mao*, and Z. Q. Tian. Organic–inorganic interactions of single crystalline organolead halide perovskites studied by Raman spectroscopy.
Phys. Chem. Chem. Phys., **2016**, 18, 18112.

[3] H. X. Lin, L. Chen, D. Y. Liu, Z. C. Lei, **Y. Wang**, X. S. Zheng, B. Ren, Z. X. Xie, Galen D. Stucky*, and Z. Q. Tian*. Constructing two-dimensional nanoparticle arrays on layered materials inspired by atomic epitaxial growth.
J. Am. Soc. Chem., **2015**, 137, 2828.

[2] **Y. Wang**, H. X. Lin, L. Chen, S. Y. Ding, Z. C. Lei, D. Y. Liu, X. Y. Cao*, H. J. Liang, Y. B. Jiang, and Z. Q. Tian*. What molecular assembly can learn from catalytic chemistry.
Chem. Soc. Rev., **2014**, 43, 399.

[1] **Y. Wang**, H. X. Lin, S. Y. Ding, D. Y. Liu, L. Chen, Z. C. Lei, F. R. Fan, and Z. Q. Tian*. Some thoughts about controllable assembly (I) — From catalysis to catassembly.
Sci. Sin. Chim., **2012**, 4, 525.