Guorong Weng

Macau Institute of Materials Science and Engineering
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Google Scholar Profile

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Education

University of California, Santa Barbara 09/2018 – 06/2023
Ph.D. in Chemistry *Santa Barbara, CA*

Zhejiang University 09/2014 – 06/2018
B.Sc. in Chemistry *Hangzhou, Zhejiang, China*

Work Experiences

Assistant Professor 01/2026 – Present
Macau University of Science and Technology *Taipa, Macau*

Postdoctoral Researcher 07/2023 – 12/2025
University of California, Los Angeles *Los Angeles, CA*

Advisor: Prof. Anastassia N. Alexandrova

Research Experiences

Topological Materials in Catalysis 07/2023 – 12/2025
University of California, Los Angeles *Los Angeles, CA*

Advisor: Prof. Anastassia N. Alexandrova

- electrode materials screening and simulation
- surface state evolution under reaction conditions
- surface reconstructions and their effects on topological surface states

Stochastic Electronic Structure Theory 12/2018 – 06/2023
University of California, Santa Barbara *Santa Barbara, CA*

Advisor: Prof. Vojtěch Vlček

- simulating condensed-phase systems
- developing low-scaling quantum mechanical methods
- investigating excited-state dynamics and electronic couplings

Hole-Transport Materials in Perovskite Solar Cells 10/2017 – 06/2018
Zhejiang University *Hangzhou, Zhejiang, China*

Advisor: Prof. Peng Wang

- synthesis of organic semiconducting molecules
- tests and characterizations of device performance
- spectroscopic characterizations of synthetic products

Mentoring and Teaching Experiences

Summer Research Mentor 06/2020 and 06/2021

UCSB Research Mentorship Program (RMP)

- design research projects for students admitted to RMP
- teach fundamental quantum chemical theories
- monitor research activities and progress

Program Alumni

- Rushil Mallarapu, 2020 RMP student, currently at Harvard University studying mathematics and statistics
- Amanda Pang, 2021 RMP student, currently at the University of Pennsylvania studying chemistry

Teaching Assistant 2018-2020

CHEM 1CL in Fall 2018

- general chemistry lab courses for students in the lower division
- lecturing and supervising experiments
- grading quiz and lab reports

CHEM 116 series in 2019

- physical chemistry lab courses for students in the upper division
- setting up instruments and coordinating experiments
- teaching academic writing and grading lab papers

CHEM 222 A in Fall 2020

- fundamental quantum chemistry courses for graduate students and senior undergraduate students
- designing and grading homework assignments
- leading remote discussion sessions on Zoom

Research Presentations

1. "Quasiparticle excitations and band structures in organized donor-acceptor copolymers," contributed talks at MRS Spring Meeting, ACS Spring Meeting, and APS March Meeting in 2021
2. "Efficient treatment of molecular excitations in the Liquid phase using stochastic many-body theory," contributed talks at ACS Spring Meeting and APS March Meeting in 2022
3. "Electronic structures in condensed Phase using stochastic many-body methods," Poster, ACTC in 2022
4. "Regionally Pipek-Mezey localized occupied and virtual orbitals and applications to embedding methods," contributed talk at ACS Spring Meeting in 2023
5. "Embedding vertex correction in stochastic *GW* self-energy," contributed talk at APS March Meeting in 2023
6. "Quasiparticle excitations and dynamics in the condensed phase," Poster, Workshop on Functional Materials and Organic Electronics in 2023
7. "Evolution of Surface States in Topological Materials for Electrocatalysis," Poster Talk, Gordon Research Conference: Chemical Reactions at Surfaces, 2025

8. "Sn-based Topological Semimetals for Catalysis: Bulk Topology, Boundary Correspondence, and Surface States Evolution under Reaction Conditions," Poster, Marcus Center's Inaugural Meeting, 2025

Specialized Skills

Computer Programing: Fortran, MPI, OpenMP, bash and Python
Computations: VASP, NWchem, Quantum Espresso, MACE, ase, Wannier90
Academic Writing: Latex
Research Mentoring: graduate and undergraduate student mentoring
Teaching: lecturing in general chemistry and physical chemistry labs

Research Interests

electronic structure theory, topological materials, computational catalysis, quantum embedding methods, machine-learning force-fields

Awards & Honors

AFOSR Scholar
American Conference on Theoretical Chemistry *2022*
DeWolfe Distinguished Teaching Fellow
UCSB *2022*
Summer Chair's Fellowship
UCSB *2021*
Outstanding Service to the Department
UCSB *2021*
Phi Lambda Upsilon Award
UCSB *2019*
Outstanding Graduate
Zhejiang Province *2018*
Guanghua Scholarship
Zhejiang University *2017*
Undergraduate National Scholarship
China *2016*

Publications

1. "A Low-Energy-Gap Thienochrysenocarbazole Dye for Highly Efficient Mesoscopic Titania Solar Cells: Understanding the Excited State and Charge Carrier Dynamics," J. Wang, X. Xie, **G. Weng**, Y. Yuan, J. Zhang, P. Wang, *ChemSusChem*, 2018, 11, 1460
2. "Stochastic Many-Body Perturbation Theory for Moire States in Twisted-Bilayer Phosphorene ," J. Brooks, **G. Weng**, S. Taylor, V. Vlček, *J. Phys.: Condens. Matter*, 2020, 32, 234001
3. "Quasiparticle and Band Structures in Organized Nanostructures of Donor-Acceptor Copolymers," **G. Weng**, V. Vlček, *J. Phys. Chem. Lett.*, 2020, 11, 17, 7177
4. "Efficient Treatment of Molecular Excitations in the Liquid Phase Environment via Stochastic Many-Body Theory," **G. Weng**, V. Vlček, *J. Chem. Phys.*, 2021, 155, 054104 (Editor's Choice)

5. "Are Multi-quasiparticle Interactions Important in Molecular Ionization?" C. M. Carlos, **G. Weng**, M. Romanova, S. J. Cotton, K. B. Whaley, N. Tubman, V. Vlček, *J. Chem. Phys.*, 2021, 154, 121101
6. "Reduced Scaling of Optimal Regional Orbital Localization via Sequential Exhaustion of the Single-Particle Space," **G. Weng**, M. Romanova, A. Apelian, H. Song, V. Vlček, *J. Chem. Theory Comput.*, 2022, 18, 8, 4960
7. "Dynamical downfolding for localized quantum states," M. Romanova, **G. Weng**, A. Apelian, V. Vlček, *npj Comput Mater*, 2023, 9, 126
8. "Embedding vertex corrections in *GW* self-energy: Theory, implementation, and outlook," **G. Weng**, M. Rushil, V. Vlček, *J. Chem. Phys.*, 2023, 158, 144105
9. "Spatial Decay and Limits of Quantum Solute-Solvent Interactions," **G. Weng**, A. Pang, V. Vlček, *J. Phys. Chem. Lett.*, 2023, 14, 10, 2473
10. "Understanding the Adiabatic Evolution of Surface States in Tetradymite Topological Insulators under Electrochemical Conditions," **G. Weng**, W. Laderer, Anastassia N. Alexandrova, *J. Phys. Chem. Lett.*, 2024, 15, 10, 2732
11. "Understanding the Finite Size and Surface Relaxation Effects on the Surface States of Bi_2Se_3 Family Topological Insulators," **G. Weng**, Anastassia N. Alexandrova, *J. Phys. Chem. C.*, 2024, 128, 48, 20659
12. "Unravelling the Surface Termination and Evolution of Surface States for Electrocatalyst $PtSn_4$ in Alkaline HER," **G. Weng**, Anastassia N. Alexandrova, *ACS Catal.*, 2025, 15, 12, 10448
13. "Bulk-Boundary Correspondence of Semimetal Ru_3Sn_7 and Topological Surface States on Chemically Realistic Terminations," **G. Weng**, Anastassia N. Alexandrova, *Adv. Mater. Interfaces*, 2025, e00711