

PHYSICAL CHEMISTRY SEMINAR

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Advancing Computational Design of Electrocatalysts for Hydrogen Fuel Cells and Water Electrolysis

The research in my group focuses on discovering, designing and developing electrocatalysts with improved performance for hydrogen fuel cells and water electrolysis, including the hydrogen evolution and oxidation reaction reactions (HER/HOR) at the metal/oxide interfaces, the oxygen reduction reaction (ORR) on platinum group metal (PGM) surfaces and the oxygen evolution reaction (OER) on transition metal oxides. In the presentation, I will review our work in the strain engineering of PGM for ORR and the active sites of OER on Ni-based oxyhydroxides.

The strain effect is one of the well-known factors that promotes ORR activity. What is unknown, at least unclear, is how to effectively generate and tune surface strain. In this seminar, I will introduce three strategies for strain generation and tuning, including intrinsic strain[1], atomic site-specific strain,[2] and critical strain.[3]

Regarding OER on Ni-based oxyhydroxides, despite over five decades of research, the atomic-scale structures of the active phases remain elusive, hindering the identification of active sites. In this seminar, I will provide direct atomic-scale insights into their crystal structures and structural transformations, shedding light on unique active sites: synergistic dual-metal reaction centers.[4-7]

1. Wang, L.; Zeng, Z.; Gao, W.; Maxson, T.; Raciti, D.; Giroux, M.; Pan, X.; Wang, C.; Greeley, J. *Science* **2019,** 363, (6429), 870-874.
2. Liu, G.; Shih, A. J.; Deng, H.; Ojha, K.; Chen, X.; Luo, M.; McCrum, I. T.; Koper, M. T. M.; Greeley, J.; Zeng, Z. *Nature* **2024,** 626, (8001), 1005-1010.
3. Zeng, Z.; Liu, G.; Cullen, D. A.; Deng, H.; Steinbach, A. J.; Thoma, G. M.; Jeremy Kropf, A.; Myers, D. J.; Shang, Z.; Kusaka, F.; Todoroki, N.; Greeley, J. P. *Nature Energy* **2026,** 11, 1437-1448.
4. Dionigi, F.; Zeng, Z.; Sinev, I.; Merzdorf, T.; Deshpande, S.; Lopez, M. B.; Kunze, S.; Zegkinoglou, I.; Sarodnik, H.; Fan, D.; Bergmann, A.; Drnec, J.; Araujo, J. F. d.; Gliech, M.; Teschner, D.; Zhu, J.; Li, W.-X.; Greeley, J.; Cuenya, B. R.; Strasser, P. *Nature Communications* **2020,** 11, (1), 2522.
5. Dionigi, F.; Zhu, J.; Zeng, Z.; Merzdorf, T.; Sarodnik, H.; Gliech, M.; Pan, L.; Li, W.-X.; Greeley, J.; Strasser, P. *Angew. Chem., Int. Ed.* **2021,** 60, (26), 14446-14457.
6. Klingenhof, M.; Trzesniowski, H.; Koch, S.; Zhu, J.; Zeng, Z.; Metzler, L.; Klinger, A.; Elshamy, M.; Lehmann, F.; Buchheister, P. W.; Weisser, A.; Schmid, G.; Vierrath, S.; Dionigi, F.; Strasser, P. *Nature Catalysis* **2024,** 7, (11), 1213-1222.
7. Choi, D.; Buchheister, P. W.; Somaiya, R.; Ligay, D.; Podbielski, G.; Lu, J.; Schröer, P.; Bumenn, E.; Galkina, I.; Scheepers, F.; Brejwo, Z.; Hartmann, A.; Paul, B.; Thanh, T. N.; Klingenhof, M.; Karl, A.; Jodat, E.; Eichel, R. A.; Zeng, Z.; Dionigi, F.; Strasser, P. *J. Am. Chem. Soc.* **2026,** 148, 40198-40212.

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Zhenhua Zeng's Biography

Dr. Zeng is an assistant research professor in the Tarpo Department of Chemistry at Purdue University with courtesy appointment in the School of Materials Engineering and Institute of Physics AI. His research focuses on first-principles-based modeling of catalysts and interfaces for hydrogen fuel cells and water electrolysis. Dr. Zhenhua Zeng obtained his a BS degree in Applied Physics and a Master's degree in Materials Science from Hunan University (China). He obtained his Ph.D. degree in Physical Chemistry from the Dalian Institute of Chemical Physics, the Chinese Academy of Sciences. He had his first postdoctoral training at the Technical University of Denmark. Then, he moved to Argonne National Laboratory, before joining Purdue. Dr. Zeng has published over 60 peer-reviewed papers (13k+citations), including those in Nature and Science as a corresponding author. Dr. Zeng was a winner of the 2019-2020 ECS Toyota Young Investigator Fellowships.