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Department of Chemistry

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Via: MS TEAMS

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First-Principles Simulations of Electrocatalysis and Electron Transport

ABSTRACT: Computational methods based on quantum mechanics (first principles) are powerful tools to extract atomic-level understanding of materials and processes, which may be difficult to access experimentally. Here I will show two examples, where we use first-principles methods to understand (1) the active site structure and the mechanism of electrochemical carbon dioxide reduction catalyzed by single nickel atom embedded in graphene. This catalyst has shown high activity and selectivity for carbon dioxide reduction while the active site structure and the mechanism are under debate. We find that the charge capacity, a previously-overlooked factor, is the key in determining the catalytic performance of different sites [1,2,3]; (2) why 2D semiconductors, despite their promise for next-generation electronics, generally have low electron mobility at room temperature. We find that the universally low mobility of 2D semiconductors originates from the high "density of scatterings," which is intrinsic to the 2D material with a parabolic electron band. The density of scatterings characterizes the density of phonons that can interact with the electrons and can be fully determined from the electron and phonon band structures without knowledge of electron-phonon coupling strength, offering a descriptor to quickly assess the mobility [4,5,6].

References

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BIO:

Yuanyue Liu is currently an assistant professor at Department of Mechanical Engineering and Texas Materials Institute at University of Texas at Austin. He received B.S. degree from University of Science and Technology of China (USTC) in 2008, and Ph.D. from Rice University in 2014. He did postdoc studies at National Renewable Energy Laboratory (NREL) and California Institute of Technology, and then joined UT in Fall 2017. He has received a number of awards, including Scialog Fellow, Computational Materials Science Rising Stars Finalist, J. Mat. Chem. A Emerging Investigator, J. Phys. Mater. Emerging Leader, ACS PRF New Doctoral Investigator, Resnick Prize Postdoc Fellowship, and Franz and Frances Brotzen Award. He has been cited > 8500 times.