

Professor LI, YOUYONG

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Academic Qualification

Ph.D. in Chemistry, California Institute of Technology

M.S. in Chemistry, Peking University

B.S. in Chemistry, Peking University

Teaching Area

Materials simulation and Design

Computational Chemistry

Research Area

Energy materials and Catalytic materials

Materials simulation and Design

Computational Chemistry

Working Experience

2005-2005, Postdoctoral Researcher, California Institute of Technology

2006-2009, Research Staff, California Institute of Technology

2009, Professor, Soochow University

2021-present, Professor, Macau University of Science and Technology

Academic Publication

Xing Fan, Siyu Tan, Junjun Yang, Yunxia Liu, Wenyi Bian, Fan Liao*, Haiping Lin*, **Youyong Li***, "From Theory to Experiment: Cascading of Thermocatalysis and Electrolysis in Oxygen Evolution Reactions", ACS Ener. Lett., 2022, 7, 343.

Siyu Tan, Yujin Ji*, and **Youyong Li***, "Single-Atom Electrocatalysis for Hydrogen Evolution Based on the Constant Charge and Constant Potential Models", J. Phys. Chem. Lett. 2022, 13, 30, 7036–7042.

Ningning Kong, Xing Fan, Fangfang Liu, Lu Wang, Haiping Lin,* **Youyong Li,*** and Shuit-Tong Lee, "Single Vanadium Atoms Anchored on Graphitic Carbon Nitride as a High-Performance Catalyst for Non-Oxidative Propane Dehydrogenation", ACS Nano, 2020, 14, 5772-5779.

Lu Wang*, Hai Xiao, Tao Cheng, **Youyong Li***, William A. Goddard III*, " Pb-activated Amine-assisted Photocatalytic Hydrogen Evolution Re-action on Organic-Inorganic Perovskites ", J. Am. Chem. Soc., 2018, 140, 1994-1997

Yunzhou Wen, Cheng Liu, Rui Huang, Hui Zhang, Xiaobao Li, F. Pelayo García de Arquer, Zhi Liu, **Youyong Li***, Bo Zhang*, "Introducing Brønsted acid sites to accelerate the bridging-oxygen-assisted deprotonation in acidic water oxidation", Nature Communications, 2022, 13, 1-11.

Books

Yujin Ji, Xiaojuan Xu, Tingjun Hou, **Youyong Li**, "Characterizing the Morphology and Efficiency of Organic Solar Cells by Multiscale Simulations", S. Shankar et al. (eds.), Computational Materials, Chemistry, and Biochemistry: From Bold Initiatives to the Last Mile, Springer Series in Materials Science 284

Xiaotian Sun, Zhiwei Feng, Tingjun Hou, **Youyong Li**, "Computational simulation of inorganic nano-particle drug delivery systems at the molecular level" of "Computational Pharmaceutics: Application of Molecular Modeling in Drug Delivery", Wiley, 2015

Patents

US Patent, (WO/2008/097560) "Methods for the Identification of Drugs that Interact with the G Protein Coupled Receptor DP", Inventors: William A. Goddard III, Nagarajan Vaidehi, **Youyong Li**, et al.

Professional Certification and Awards

Global highly cited scientist of Clarivate in 2020, 2021, 2022
First prize of Jiangsu Science and Technology Award in 2017

Student Awards

N/A

Professional Society Membership

Member of computational chemistry committee of Chinese Chemical Society
Editorial Board Member of "Scientific Reports"
Editorial Board Member of "Frontiers in Materials"