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Accelerating the photocatalytic water splitting in catalyst-dye complexes

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List of Publications

Main Publications:

- **Yang Shao**, Jessica M. de Ruiter, Huub J.M. de Groot, and Francesco Buda, Photocatalytic Water Splitting Cycle in a Dye–Catalyst Supramolecular Complex: *Ab Initio* Molecular Dynamics Simulations, *J. Phys. Chem. C*, **2019**, 123, 21403–21414. DOI: 10.1021/acs.jpcc.9b06401 (**Chapter 2**)
- **Yang Shao**, Huub J.M. de Groot, and Francesco Buda, Proton Acceptor near the Active Site Lowers Dramatically the O–O Bond Formation Energy Barrier in Photocatalytic Water Splitting, *J. Phys. Chem. Lett.*, **2019**, 10, 7690–7697. DOI: 10.1021/acs.jpclett.9b02914 (**Chapter 3**)
- **Yang Shao**, Huub J.M. de Groot, and Francesco Buda, Tuning the Proton-Coupled Electron-Transfer Rate by Ligand Modification in Catalyst–Dye Supramolecular Complexes for Photocatalytic Water Splitting, *ChemSusChem*, **2021**, 14, 479–486. (Featured as VIP paper)
DOI: 10.1002/cssc.202001863 (**Chapter 4**)
- **Yang Shao**, Huub J.M. de Groot, and Francesco Buda, Two-Channel Model for Electron Transfer in a Dye–Catalyst–Dye Supramolecular Complex, **2021**, manuscript to be submitted. (**Chapter 5**)

Other publications not included in this thesis:

- Xuequan Zhou, Maria Mytiliniou, Jonathan Hilgendorf, Ye Zeng, Panagiota Papadopoulou, **Yang Shao**, Erik Bos, Maxime A. Siegler, Francesco Buda, Alexander Kros, Roman I. Koning, Doris Heinrich, and Sylvestre Bonnet, Intracellular dynamic assembly of deep-red-emitting supramolecular nanostructures based on Pt...Pt metallophilic interaction, **2021**, submitted.
- Xuequan Zhou, Wen Sun, Peiyuan Wang, Vadde Ramu, Suhua Jiang, Selda Abyar, Panagiota Papadopoulou, **Yang Shao**, Maxime A Siegler, Francesco Buda, Alexander Kros, Sylvestre Bonnet, Self-assembling Cyclopalladated Photosensitizers for Photodynamic Therapy: Tumor Accumulation and Anti-tumor Activity in a Skin Melanoma Xenograft, **2021**, manuscript in preparation.
- Xiaoqing Lu,[†] **Yang Shao**,[†] Ke Li, Zigang Zhao, Shuxian Wei, and Wenyue Guo, Role of Functionalized Acceptors in Heteroleptic Bipyridyl Cu(I) Complexes for Dye-Sensitized Solar Cells, *Electron. Mater. Lett.*, **2016**, 12, 589–595. DOI: 10.1007/s13391-016-6035-z. ([†]Both authors contributed equally.)

- Shuxian Wei, **Yang Shao**, Xiaofan Shi, Xiaoqing Lu, Ke Li, Zigang Zhao, Chen Guo, Houyu Zhu, and Wenyue Guo, Heteroleptic Cu (I) Complexes Integrating Functionalized Chromophores for Dye-Sensitized Solar Cells: An In-depth Analysis of Electronic Structure, Spectrum, Excitation, and Intramolecular Electron Transfer. *Org. Electron.*, **2016**, 29, 142-150. DOI: 10.1016/j.orgel.2015.12.004.
- Shuxian Wei, Ke Li, Xiaoqing Lu, Zigang Zhao, **Yang Shao**, Yong Dang, Shaoren Li, and Wenyue Guo, Theoretical Insight into Electronic Structure and Optoelectronic Properties of Heteroleptic Cu(I)-based Complexes for Dye-Sensitized Solar Cells. *Mater. Chem. Phys.*, **2016**, 173, 139-145. DOI: 10.1016/j.matchemphys.2016.01.049.
- **Yang Shao**, Xiaoqing Lu, Ke Li, Zigang Zhao, Xiaofan Shi, Dongliang Jin, Houyu Zhu, Guangwu Yang, and Wenyue Guo, Theoretical Insight into Photo-induced Intramolecular Electron Transfer in Heterodinuclear Ru(II)-Co(III) complexes, *Mater. Chem. Phys.*, **2015**, 162, 6-10. DOI: 10.1016/j.matchemphys.2015.05.041.
- Xiaoqing Lu,[†] **Yang Shao**,[†] Shuxian Wei, Zigang Zhao, Ke Li, Chen Guo, Weili Wang, Mingmin Zhang, and Wenyue Guo, Effect of the Functionalized π -bridge on Porphyrin Sensitizers for Dye-Sensitized Solar Cells: an In-depth Analysis of Electronic structure, Spectrum, Excitation, and Intramolecular Electron Transfer. *J. Mater. Chem. C*, **2015**, 3, 10129-10139. DOI: 10.1039/C5TC02286J. ([†]Both authors contributed equally.)
- Kunpeng Guo, Zhixiang Gao, Jun Cheng, **Yang Shao**, Xiaoqing Lu, and Hua Wang, Linear Thiophene-containing π -conjugated Aldehydes with Aggregation-induced Emission for Building Solid Red Luminophors. *Dyes Pigm.*, **2015**, 115, 166-171. DOI: 10.1016/j.dyepig.2014.12.017.
- Shuxian Wei, Xiaofan Shi, Xiaoqing Lu, **Yang Shao**, Dongliang Jin, Zhigang Deng, Zigang Zhao, Ke Li, and Wenyue Guo, Cu(I)-Based Sensitizers Featuring 6,6'-Dimethyl-4,4'-Dicarboxylate-2,2'-Bipyridine with Functionalized 2,9-Dimethyl-1,10-Phenanthroline Ligands: A Structural, Electronic and Spectral Investigation. *Sci. Adv. Mater.*, **2015**, 7, 1361-1367. DOI: 10.1166/sam.2015.2052.
- Xiaoqing Lu, Weili Wang, Shuxian Wei, Chen Guo, **Yang Shao**, Mingmin Zhang, Zhigang Deng, Houyu Zhu, and Wenyue Guo, Initial Reduction of CO₂ on Perfect and O-defective CeO₂(111) Surfaces: Towards CO or COOH? *RSC adv.*, **2015**, 5, 97528-97535. DOI: 10.1039/C5RA17825H.
- Xiaofan Shi, Xiaoqing Lu, **Yang Shao**, Shuxian Wei, Qing Zhu, Dongliang Jin, Zhigang Deng, and Wenyue Guo, Theoretical Investigation on Novel Porphyrin Dyes with Functionalized Bridge and Donor Groups for Dye-Sensitized Solar Cells. *Sci. Adv. Mater.*, **2014**, 6, 2595-2602. DOI: 10.1166/sam.2014.2007.
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Curriculum Vitae

Yang Shao was born on March 10th, 1990 in the north-central part of Shandong province, China. He grew up in a county-level city – Shouguang, the “home of vegetables” in China, located on an alluvial plain drained by the Mihe River that flows down from Qingzhou city. It stretches to the Bohai Sea, where you can conquer a mountain in one step, since Jing Mountain is the only mountain in Shouguang and at the same time the smallest mountain in China. It measures at just 60 cm high and 70 cm wide, and yet is not classified as a rock.

In 2009, he went to Dongying city, which is in the same Shandong province, and enrolled as a bachelor student at China University of Petroleum to study materials physics. In 2011, he moved to the new university campus in Qingdao, where he developed an interest in solar cells and obtained his bachelor degree in 2013. Successively, he joined the New Energy Materials Group as a recommended candidate to perform computational research under the supervision of Prof. dr. Wen Yue Guo and Prof. dr. Xiaoqing Lu (currently the leader of New Energy and Environmental Science Group), where he started his master research on dye-sensitized solar cells by means of DFT calculations. In 2016, he obtained his master degree in Materials Engineering and was rated as “Outstanding Graduate Student of Shandong Province”.

In September 2016, thanks to the funding from Chinese Scholarship Council (CSC), he moved to Leiden, the Netherlands, and started his PhD project under the supervision of Dr. Francesco Buda and Prof. dr. Huub de Groot at Leiden Institute of Chemistry, Leiden University. During his PhD research in the field of artificial photosynthetic water splitting, he extended his research skills to DFT-based *ab initio* molecular and finite element simulations. He also wrote codes with Python to assist in data analysis. In the time of his PhD he gave poster presentations at the Holland Research School of Molecular Chemistry (HRSMC) Annual Symposium (UvA, 2017), Reedijk Symposium (LU, 2018), Royal Dutch Chemical Association (KNCV) Division Computational & Theoretical Chemistry (VU, 2019). In addition, part of his work has been selected to be orally presented at the International Union of Pure and Applied Chemistry (IUPAC) (Paris, 2019) and Chemistry as Innovating Science (CHAINS) (Eindhoven, 2019).

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