Curriculum vitae Pengbo Lyu

Current Position:

PhD study – Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University

Study program: Modeling of Chemical Properties of Nano- and Biostructures
Courses: reactivity modeling, quantum chemistry and advanced physical chemistry.
Thesis theme: Theoretical investigation of adsorption and catalytic properties of novel materials
PhD supervisor: Prof. Petr Nachtigall
PhD Advisor: Lukas Grajciar

Summary of PhD research project:

I started the research from the mechanism of hydrodeoxygenation of phenol over nickel phosphide surface to explain the observation from our experimental collaborators, and then spent some time on the theoretical study of CO oxidation catalysts. Then I focus on the hydrolysis of Ge-substituted UTL zeolite and tetrahydropyranylation mechanisms in porous materials. After that I worked on the structures of 2D materials (such as LDH, COFs and silicene) and their applications in collaboration with experimentalists and got some good publications. I also have some publications on spintronics in collaboration with my former colleague, Junjie He. I have a grant from Grant Agency of Charles University (GAUK) (Grant No. 1392217) for photocatalytic applications of LDHs and now I am still working on it. I also have some experience in calculation of oxygen evolution reaction (OER) with descriptors.

Work Experience:

2010-2013 Worked as a chemistry teacher and part-time lab technician in Yongjia High School, Wenzhou, China

Education and Academic Degree:

2006-2010 Undergraduate studies : College of Chemistry and Materials Science, Shannxi Normal University

2013-2015 Study for a master degree in science in Department of Chemistry, School of Science, Harbin Institute of Technology. Advisor: Prof. Li Sheng , Master thesis title: Density Functional Theory Study of the mechanism of the conversion of CO_2 and CH_4 to CH_3COOH over Zn/ZSM-5 catalysts

2015-now Doctoral study in Charles University

Publications:

Total of 14 papers, 14 out of them during PhD study (since 2015). In addition, one manuscript was submitted and two are in preparation.

Papers (published during PhD study, from 2015):

1. J. J. Liu, **P. B. Lyu**, Y. Zhang, P. Nachtigall, Y. X. Xu, New Layered Triazine Framework/Exfoliated 2D Polymer with Superior Sodium-Storage Properties, Adv. Mater. 2018, 30, 1705401. (co-first author)
2. J. J. Liu, Y. Yang, **P. B. Lyu**, P. Nachtigall, Y. X. Xu, Few-Layer Silicene Nanosheets with Superior Lithium-Storage Properties, Adv. Mater. 2018, 1800838.
3. Haiyan Duan, **Pengbo Lyu**, Jingjing Liu, Yanli Zhao, and Yuxi Xu, Semiconducting Crystalline Two-Dimensional Polyimide Nanosheets with Superior Sodium Storage Properties, *ACS Nano 2019, 13, 2, 2473-2480*
4. **Pengbo Lyu**, Junjie He and Petr Nachtigall, "Theoretical investigation of CO catalytic oxidation by a Fe–PtSe2 monolayer", RSC Adv., 2017, 7, 19630-19638
5. S. Gong, G. Zhao, **P. Lyu**, K. Sun, A Pseudolayered MoS_2 as Li-Ion Intercalation Host with Enhanced Rate Capability and Durability, *Small* 2018, 14, 1803344
6. S. Gong, G. Zhao, **P. Lyu**, K. Sun, Insights into the intrinsic capacity of interlayer-expanded MoS2 as a Li-ion intercalation host, J. Mater. Chem. A, 2019,7, 1187-1195
7. Mingxiu Liu, Ondřej Veselý, Pavla Eliášová, Mariya Shamzhy, Lukáš Grajciar and **Pengbo Lyu**, Identification

of the Most Active Sites for Tetrahydropyranylation in Zeolites: MFI as a test case, *submitted*

8. **Pengbo Lyu** and Petr Nachtigall, Tuning the Band Gap of CTF-type COFs for Photocatalytic Water Splitting Potential: Computational Investigation, *in preparation*
9. **Pengbo Lyu**, Christopher J. Heard, Lukáš Grajciar, Michael Ertl, Josef Breu, Petr Nachtigall, The Structure of Layered Double Hydroxides of the Fougèrite Group: combined experimental and theoretical investigation, *in preparation*
10. Jan Engelhardt, **Pengbo Lyu**, Petr Nachtigall, Ferdi Schüth and Ángel Morales García, The Influence of Water on the Performance of Molybdenum Carbide Catalysts in Hydrodeoxygenation Reactions: A Combined Theoretical and Experimental Study, *ChemCatChem* 2017, *9*, 1985.
11. Dana Schwarz, Amitava Acharja, Arun Ichangi, **Pengbo Lyu**, Maksym V. Opanasenko, Fabian R. Goßler, Tobias A. F. König, Jiří Čejka, Petr Nachtigall, Arne Thomas, Michael J. Bojdys, "Fluorescent sulphur and nitrogen containing porous polymers with tuneable donor-acceptor domains for light-driven hydrogen evolution*", Chem. Eur. J.* 2018, 24, 11916.
12. Schwarz, D. , Acharjya, A. , Ichangi, A. , Kochergin, Y. S., **Lyu, P**. , Opanasenko, M. V., Tarábek, J. , Vacek Chocholoušová, J. , Vacek, J. , Schmidt, J. , Čejka, J. , Nachtigall, P. , Thomas, A. and Bojdys, M. J. (2018), Tuning the Porosity and Photocatalytic Performance of Triazine‐Based Graphdiyne Polymers through Polymorphism, *ChemSusChem* **2019**, *12*, 194.
13. Junjie He, **Pengbo Lyu**, Lizhong Sun, Angel Morales-Garcia, and Petr Nachtigall. "Two-dimensional Janus MXenes: High-temperature Spin-polarized Semiconductor with Zero Magnetization." Journal of Materials Chemistry C, 4, (2016), 6500-6509.
14. Junjie He, Shuangying Ma, **Pengbo Lyu**, and Petr Nachtigall. "Unusual Dirac half-metallicity with intrinsic ferromagnetism in vanadium trihalide monolayers." Journal of Materials Chemistry C 4, (2016): 2518-2526.
15. Junjie He , **Pengbo Lyu** and Petr Nachtigall," New Two-Dimensional Mn-based MXenes with Room-Temperature Ferromagnetism and Half-Metallicity", J. Mater. Chem. C, 2016, 4, 11143-11149
16. Junjie He, Xiao Li, **Pengbo Lyu** and Petr Nachtigall, Near-room-temperature Chern insulator and Dirac spin-gapless semiconductor: nickel chloride monolayer, Nanoscale, 2017, 9, 2246-2252
17. Junjie He, **Pengbo Lyu**, Petr Nachtigall, Two-dimensional tetragonal GaOI and InOI sheets: In-plane anisotropic optical properties and application to photocatalytic water splitting, *Catalysis Today*, https://doi.org/10.1016/j.cattod.2018.10.012

Conference:

The 2016 CAMD Summer School on Electronic Structure Theory and Materials Design, Kongens Lyngby, Denmark poster, title:A Theoretical Investigation of Hydrodeoxygenation of Phenol over Nickel Phosphide

CASCATBEL workshop, 18-20 May,2016, Chalkidiki, Greece, poster, A Theoretical Investigation of Hydrodeoxygenation of Phenol over Nickel Phosphide, Pengbo Lyu, Junjie He, Petr Nachtigall

47th Symposium on Catalysis, 2-4 November 2015, 47th Symposium on Catalysis, ÚFCH J. Heyrovského AVČR poster, Junjie He, Pengbo Lyu, Ángel Morales-García, and Petr Nachtigall,Understanding the HDO reaction of phenol molecule on Ni2P and Mo2C surfaces. A computational study.

21-22 March, 2016, School on Layered Materials, ÚFCH J. Heyrovský ho AVČR (Prague), poster, A theoretical investigation of Fe embedded monolayer PtSe2 for CO catalytic oxidation, Pengbo Lyu, Junjie He, Petr Nachtigall

48th Symposium on Catalysis, 2-4 November 2015, 47th Symposium on Catalysis, ÚFCH J. Heyrovského AVČR, oral presentation, Pengbo Lyu, Junjie He, Ángel Morales-García, and Petr Nachtigall, A Theoretical Investigation of Hydrodeoxygenation of Phenol over Nickel Phosphide

Electronic Structure: Principles and Applications (ESPA 2016) Castellón, Spain, poster, title: A theoretical investigation of Fe embedded monolayer PtSe2 for CO catalytic oxidation

11th European Coference on Theoretical and Computational Chemistry, poster, Pengbo Lyu, Junjie He and Petr Natichgall, Theoretical investigation of CO catalytic oxidation by Fe-PtSe2 monolayer

6th European Conference on Molecular Magnetism, Junjie He, Xiao Li, Pengbo Lyu and Petr Nachtigall, Prediction of intrinsic quantum anomalous Hall states with high-temperature ferromagnetism in Nickle chloride monolayer

7th Czech-Italian-Spanish Symposium on Catalysis, poster, Pengbo Lyu, Zhengwen Cao, Junjie He, Petr Nachtigall, A Theoretical Investigation of Hydrodeoxygenation of Phenol over Nickel Phosphide

Lecture Series on Materials Theory and Computation, 28th June-2 July 2018, Xi'an Jiaotong University, Poster, Pengbo Lyu and Petr Nachtigall, Theoretical investigation of COF stacking and effects on photocatalysis