Liangxu XIE

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EDUCATION

Ph.D., Department of Chemistry, the University of Hong Kong, 2016
Major: Computational Chemistry
Concentration: Molecular dynamics simulation for biomolecules and polymers
Thesis: Molecular Dynamics Simulations of Thermodynamic Properties of Selected Polymeric and Biological Molecules
Thesis Supervisor: Kwong-Yu Chan

B.Sc, School of Chemistry and Chemical Engineering, Shandong University, 2011

RESEARCH EXPERIENCE

Associate Professor, Jiangsu University of Technology, 2019-
Research area: Multi-scale modeling and deep learning

Research Associate, Hong Kong University of Science and Technology, 2017-2018
Research area: Virtual screening of drug molecules with free energy calculation methods and deep learning
Supervisor: Xuhui Huang

Research Assistant, the University of Hong Kong, 2016-2017
Research area: Molecular dynamics simulation for polyelectrolyte~MOF composite
Supervisor: Kwong-Yu Chan

PUBLICATIONS

1. **Liangxu Xie,** Lei Xu, Ren Kong, Shan Chang*，and Xiaojun Xu*；Improvement of Prediction Performance with Conjoint Molecular Fingerprint in Deep Learning； ***Front. Pharmacol.***；2020, 11, 606668
2. **Liangxu Xie#*,** Lei Xu#*, Shan Chang, Xiaojun Xu, Li Meng, Multitask Deep Networks with Grid Featurization Achieve Improved Scoring Performance for Protein-Ligand Binding, ***Chem. Biol. Drug Des.,*** 2020, 96(3), 973-983

3. Lei Xu,#,*, Lilei Sun,#, **Liangxu Xie**,#, Shanzhi Mou, Dawei Zhang, Jingyu Zhu, and Peng Xu, Advances in L-Type Calcium Channel Structures, Functions and Molecular Modeling; ***Curr. Med. Chem.***, 2020, 27, 1-11
4. Zhengliang Yin, **Liangxu Xie,** Shunsheng Cao*, Yingguan Xiao, Gang Chen, Ying Jiang, Wenxian Wei, Limin Wu*, Ag/Ag2O confined visible-light driven catalyst for highly efficient selective hydrogenation of nitroarenes in pure water medium at room temperature. ***Chem. Eng. J.,*** 2020, 394, 125036
5. Sai Zhang, Zhengliang Yin, **Liangxu Xie,** Jianjian Yi, Wenjie Tang, Tao Tang, Jinyu Chen, Shunsheng Cao*; Facet engineered TiO2 hollow sphere for the visible-light-mediated degradation of antibiotics via ligand-to-metal charge transfer, ***Ceram. Int.***, 2020,46(7), 8949-8957
6. **Liangxu Xie,** Huimin Cheng, Dong Fang, Zhe-Ning Chen*, Mingjun Yang*; Enhanced QM/MM Sampling for Free Energy Calculation of Chemical Reactions: A Case Study of Double Proton Transfer, ***J. Chem. Phys.*** 2019, 150, 044111
7. **Liangxu Xie,** Mingjun Yang*, Zhe-Ning Chen*, Understanding the Entropic Effect in Chorismate Mutase Reaction Catalyzed by Isochorismate-Pyruvate Lyase from Pseudomonas aeruginosa (PchB), ***Catal. Sci. Technol.*** 2019, 9, 957-965
8. Lin Wang, Junjian Chen, Xiangze Zeng, Peter Pak-Hang Cheung, Xiaoyan Zheng, **Liangxu Xie**, Xuetao Shi, Li Ren*, Xuhui Huang*, Yinjun Wang*; Mechanistic Insights and Rational Design of a Versatile Surface with Cells/Bacteria Recognition Capability via Orientated Fusion Peptides***. Adv. Sci.*** 2019, 180, 1827
9. Liang Gao, Kwong-Yu Chan*, Chi-Ying Vanessa Li, **Liangxu Xie**, Joseph Funso Olorunyomi, Highly Selective Transport of Alkali Metal Ions by Nano-channels of Polyelectrolyte Threaded MIL-53 Metal Organic Framework; ***Nano Lett.*** 2019, 19, 4990-4996
10. Tu, Zhihui, Yin, Jian, **Xie, Liangxu*;** Isotopic Effect in Double Proton Transfer Process of Porphycene Investigated by Enhanced QM/MM Method. ***J. Vis. Exp.*** 2019, (149) e60040
11. Yu Zhou, Chen Li, Jianzhao Peng, **Liangxu Xie**, Ling Meng, Jianfu Zhang, Xiang Li, Xin Li*, Xuhui Huang*, Xiaoyu Li*, DNA-encoded Dynamic Chemical Library and Its Applications in Ligand Discovery***. J. Am. Chem. Soc.*** 2018, **140,** 15859-15867
12. **Liangxu Xie,** Kwong-Yu Chan*, Nick Quirke; Poly(ethylene glycol) (PEG) in a Polyethylene (PE) Framework: A Simple Model for Simulation Studies of a Soluble Polymer in an Open Framework. ***Langmuir***; 2017, 33, 11746-11753
13. **Liangxu Xie,** Lin Shen, Zhe-Ning Chen*, Mingjun Yang*; Efficient Free Energy Calculations by Combining Two Complementary Tempering Sampling Methods. ***J. Chem. Phys.*** 2017, 146, 024103

14. Lin Shen#, **Liangxu Xie#,** Mingjun Yang*, Thermodynamic Properties of Solvated Peptides from Selective Integrated Tempering Sampling with a New Weighting Factor Estimation Algorithm. ***Mol. Phys.*** 2017, 7， 885-894

15. Liangxu Xie, Zhe-Ning Chen*, Enhanced Molecular Dynamics Simulation of the Transformation between α-helix and β-hairpin Structures for Peptide. ***Mol. Phys.*** 2016, 114，2424-2431

16. Liangxu Xie, Dongju Zhang*, Xuejiao Liu, Xi Zhang, Panpan Duan, Double Bond Isomerization of Butene Catalyzed by 1-ethyl-3-methyl-imidazolium Chloride: Concerted or Stepwise Mechanism? ***Comp. Theor. Chem***. 2011, 963, 344-347

GRANTS AND FELLOWSHIPS

1. National Natural Science Foundation of China (国家自然科学基金项目：22003020), 2021-2023
2. Natural Science Foundation of Jiangsu Province (江苏省自然科学基金项目：BK20191032), 2019-2022
3. Jiangsu “Mass Innovation and Entrepreneurship” Talent Programme (Shuang Chuang Ph.D)（江苏省“双创博士”），2020-2022
4. Changzhou Sci&Tech Program (常州市重点研发项目：CJ20200045), 2020-2022
5. Open funding from Jiangsu Sino-Israel Industrial Technology Research Institute（江苏省中以产业技术研究院开放课题：JSIITRI202009），2020

RELEVANT SKILLS

Programming ability in Python and knowledge of Keras and Tensorflow programs.
Extensive knowledge of multi-scale modeling and deep learning.

Teaching EXPERIENCE

AI in Physical Chemistry