

徐龙坤

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教育经历

澳大利亚国立大学

2018.10 - 至今

博士生 专业：化学

堪培拉， 澳大利亚

- 博士论文题目：关于改进隐溶剂模型准确度以及复杂溶剂环境中静电催化的研究
- 研究兴趣1：外电场下离子液体的结构和性质
- 研究兴趣2：复杂溶剂环境中静电催化
- 研究兴趣3：改进隐溶剂模型准确度

四川大学

2015.09 – 2018.6

硕士 专业：应用化学

成都，中国

- 硕士论文题目：关于电荷转移激发态非平衡溶剂化效应的理论研究
- 研究兴趣：非平衡溶剂化以及溶剂重组能
- GPA: 3.72/4.00

青岛农业大学

2011.09 – 2015.06

本科 专业：材料化学

青岛, 中国

- 毕业论文题目: 可生物降解聚合物的合成及其在药物输运中的应用
- GPA: 3.20/4.00

工作经历

MDPI出版社

2018.07 – 2018.09

助理编辑

北京，中国

- 作为Materials和High-throughput期刊的助理编辑，我主要负责协助两个期刊审稿过程(包括寻找专家、审稿人、排版)以及特刊的建立

公开成果

- [1] Yan B Vogel, Cameron W Evans, Mattia Belotti, **Longkun Xu**, Isabella C Russell, Li-Juan Yu, Alfred KK Fung, Nicholas S Hill, Nadim Darwish, Vinicius R Gonçalves, Michelle L. Coote, K. Swaminathan Iyer and Simone Ciampi. "The Corona of A Surface Bubble Promotes Electrochemical Reactions" Nat. Commun. **2020** 11 (1), 1–8. **(First Computational Author)**
- [2] **Longkun Xu**, Ekaterina I Izgorodina and Michelle L Coote. "Ordered Solvents and Ionic Liquids Can be Harnessed for Electrostatic Catalysis" J. Am. Chem. Soc. **2020** 142 (29), 12826–12833.
- [3] **Longkun Xu** and Michelle L Coote. "Improving the Accuracy of PCM-UAHF and PCM-UAKS Calculations Using Optimized Electrostatic Scaling Factors" J. Chem. Theory Comput. **2019** 15 (12), 6958–6967.
- [4] **Longkun Xu** and Michelle L Coote. "Methods To Improve the Calculations of Solvation Model Density Solvation Free Energies and Associated Aqueous pKa Values: Comparison between Choosing an Optimal Theoretical Level, Solute Cavity Scaling, and Using Explicit Solvent Molecules" J. Phys. Chem. A. **2019** 123 (34), 7430–7438.
- [5] Ting-Jun Bi, **Long-Kun Xu**, Fan Wang and Xiang-Yuan Li. "Solvent effects for vertical absorption and emission processes in solution using a self-consistent state specific method based on constrained equilibrium thermodynamics" Phys. Chem. Chem. Phys. **2018** 20 (19), 13178–13190. **(2018 PCCP HOT Articles)**
- [6] Mei-Jun Ming, **Long-Kun Xu**, Fan Wang, Ting-Jun Bi and Xiang-Yuan Li. "Theoretical study on electronic excitation spectra: A matrix form of numerical algorithm for spectral shift" Chem. Phys. **2017** 492, 27–34.

[7] Long-Kun Xu, Ting-Jun Bi, Mei-Jun Ming, Jing-Bo Wang and Xiang-Yuan Li. "Photoinduced charge-transfer electronic excitation of tetracyanoethylene/tetramethylethylene complex in dichloromethane" Chem. Phys. Lett. 2017 679, 158-163.

[8] Ting-Jun Bi, Long-Kun Xu, Fan Wang, Mei-Jun Ming and Xiang-Yuan Li. "Solvent effects on excitation energies obtained using the state-specific TD-DFT method with a polarizable continuum model based on constrained equilibrium thermodynamics" Phys. Chem. Chem. Phys. 2017 19 (48), 32242-32252.

详情可以参考我的谷歌学术[\[paper\]](#)

🔧 专业技能

- 科学编程: Shell, Python, Fortran, 等
- 机器学习: scikit-learn, TensorFlow, 等
- 数据科学: Pandas, NumPy, SciPy, Matplotlib, MySQL, MongoDB, 等
- 论文写作: LaTeX, Word, Markdown, 等
- 计算化学:
 - 量子化学: Gaussian, ORCA, Q-Chem, GAMESS-US, Molpro, xtb, MOPAC, COSMOtherm, ADF, 等
 - 分子动力学: LAMMPS, TRAVIS, 等
 - 材料模拟: VASP, 等
 - 波函数分析: Multiwfn, 等
 - 分子可视化: GaussView, IQmol, CYLview, VMD, PyMol, Avogadro, 等
- 量子计算: 对量子计算机以及IBM quantum平台有初级的了解
- 语言: 中文(母语), 英文(雅思7.0)

♥ 获奖情况

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|-------------------------------------|-----------|
| Postgraduate Research Support | 2020 |
| HDR Fee Remission Merit Scholarship | 2018-2021 |
| ANU PhD Scholarship (International) | 2018-2021 |
| 四川大学硕士生二等奖学金 | 2015-2018 |
| 青岛农业大学海利尔奖学金 | 2013 |

📄 其他

- 美国化学会The Journal of Physical Chemistry审稿人
- 中国化学会会员
- 个人网站(英文): <https://longkunxuluke.github.io/>
- GitHub: <https://github.com/longkunxuluke/>