

EDUCATION

Australian National University

Ph.D. in Chemistry, Advisor: Prof. Michelle Coote

Canberra, Australia

October 2018–Current

Sichuan University

M.S. in Applied Chemistry, GPA: 3.72/4.00

Chengdu, China

September 2015–June 2018

- Thesis: “Theoretical study on the non-equilibrium solvation effects on the charge-transfer excited state”

Qingdao Agricultural University

B.S. in Material Chemistry, GPA: 3.20/4.00

Qingdao, China

September 2011–June 2015

- Thesis: “Synthesis of biodegradable polymers and its application in drug delivery”

EMPLOYMENT

MDPI Publisher

Assistant Editor

Beijing, China

July 2018 to September 2018

- Assistant Editor
- As an assistant editor for journals Materials and High-throughput, I helped manage the review process of the manuscript of the two journals. Also I was involved in the setting up of the special issues of the journals.

PUBLICATIONS

- [1] **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.
- [2] **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.
- [3] **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.
- [4] 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.
- [5] 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.
- [6] **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.
- [7] 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.

TEACHING

- **Teaching Assistant** at Sichuan University
Physical Chemistry

Spring 2016

SKILLS

- **Scientific Programming:** Shell, Python, Fortran
- **Machine Learning:** scikit-learn
- **Data Processing and Visualization:** Pandas, matplotlib
- **Scientific Writing:** LaTeX
- **Computational Chemistry:** Quantum Chemistry, Molecular Dynamics, Wave function Analysis

LANGUAGES

- **Chinese:** First language
- **English:** Second language, IELTS 7.0

RESEARCH INTERESTS

See more details of my research interests on <https://longkunxuluke.github.io/>

1. Electrostatic catalysis in unusual solvent environment
2. Improving the accuracy of implicit solvent models
3. Non-equilibrium solvation and solvent reorganization

SCHOLARSHIPS AND AWARDS

- | | |
|---|-----------|
| • Postgraduate Research Support | 2020 |
| • HDR Fee Remission Merit Scholarship | 2018–2021 |
| • ANU PhD Scholarship (International) | 2018–2021 |
| • Second Class Scholarship for Graduate Student | 2015–2018 |
| • Hailier Scholarship for Outstanding Students | 2013 |

OTHER ACTIVITIES

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|---|--------------|
| • Reviewer of The Journal of Physical Chemistry | 2019–Current |
| • Member of Chinese Chemical Society | 2017–Current |