

EDUCATION

Australian National University

Canberra, Australia

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

October 2018–Current

- Expected thesis: “Toward improving the accuracy of implicit solvent models and understanding the electrostatic catalysis in complex solvent environment”
- Structure and properties of ionic liquids under external electric field
- Electrostatic catalysis in complex solvent environment
- Improving the accuracy of implicit solvent models

Sichuan University

Chengdu, China

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

September 2015–June 2018

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

Qingdao Agricultural University

Qingdao, China

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

September 2011–June 2015

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

EMPLOYMENT

MDPI Publisher

Beijing, China

Assistant Editor

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] 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.

TEACHING

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

Spring 2016

SKILLS

- **Scientific Programming:** Shell, Python, Fortran, etc.
- **Machine Learning:** scikit-learn, TensorFlow, etc.
- **Data Science:** Pandas, NumPy, SciPy, Matplotlib, MySQL, MongoDB, etc.
- **Scientific Writing:** LaTeX, Word, Markdown, etc.
- **Computational Chemistry:**
 - Quantum Chemistry (Gaussian, ORCA, Q-Chem, GAMESS-US, Molpro, xtb, MOPAC, COSMOtherm, ADF, etc.)
 - Molecular Dynamics (LAMMPS, TRAVIS, etc.)
 - Material Modelling (VASP, etc.)
 - Wave Function Analysis (Multiwfn, etc.)
 - Molecular Visualization (GaussView, IQmol, CYLview, VMD, PyMol, Avogadro, etc.)
- **Quantum Computing:** basic knowledge of quantum computer and IBM quantum

LANGUAGES

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

SCHOLARSHIPS AND AWARDS

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|---|-----------|
| • 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 |