Longkun Xu

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Education

Australian National University — Canberra, Australia
Ph.D. in Chemistry, Advisor: Prof. Michelle Coote — October 2018–October 2021

- 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

Most updated and complete list of publications can be found in my google scholar.

[8] 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 Gonçales, 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)**
[7] **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.
[6] **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.
[5] **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. **(2018 PCCP HOT Articles)**
[3] 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.
[2] **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.
[1] 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 — Spring 2016
  Physical Chemistry

Skills and Knowledge Structure

- **Computational Chemistry:** I have 6 years experience with many different aspects of computational chemistry. I am familar with the following programs:
- 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.)
- **Computer Science:** I am familiar with basic knowledge of computer science including data structure and algorithm, database. I have experience with multiple programming languages including Shell, Python, Fortran, SQL, etc. My Leetcode profile can be found here.
- **Machine Learning:** I am familar with the basic theory of machine learning. I have experience with multiple machine learning platforms including scikit-learn, TensorFlow, etc.
- **Data Science:** I am familar with the basic theory of data science. I have experience with related tools including Pandas, NumPy, SciPy, Matplotlib, MySQL, MongoDB, etc.
- **Scientific Writing:** I am comfortable with writing using LaTex, Word, Markdown, etc.
- **Quantum Computing:** I have basic knowledge of quantum computer and attended a workshop of IBM quantum hosted by Prof. Ivan Kassal at the University of Sydney.

Languages

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

Scholarships and Awards

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

Other Activities

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