Longkun Xu

Website: longkunxuluke.github.io
Email: longkunx@gmail.com
LinkedIn: Longkun Xu

Education and Employment

SAIT China Lab, Samsung Electronics — Beijing, China

Engineer — May 2022–Current

Intern — December 2021–May 2022

- Develop advanced machine learning algorithms for computational material science.
- Employ both machine learning methods (e.g., GNN) and computational chemistry methods (e.g., quantum chemistry calculations and molecular dynamic simulations) for the design of novel materials (e.g., battery materials, display materials and semiconductor materials).
- Investigate the trends of industry, build collaborations and communications with top universities.

Australian National University — Canberra, Australia

Ph.D. in Computational chemistry (Full scholarship), Advisor: Prof. Michelle Coote — October 2018–April 2022

- Thesis: "Toward improving the accuracy of implicit solvent models and understanding the electrostatic catalysis in complex solvent environment"
- Five publications (see publication 5-9) including two in *JACS* and one in *Nature Communication*, research highlighted in *EurekAlert!*, *PHYS.ORG* and *Chemistry in Australia*.
- Performed polarizable molecular dynamic simulations in LAMMPS, use Numpy, Pandas and Python scripts to analyse the MD trajectory and to study structure and properties of ionic liquids under external electric field, which is related with the choice of ionic liquids for the design of electrochemical devices, see publication 9.
- Employed computational chemistry methods (both MD simulation and quantum chemistry calculations) at different scales to study electrostatic catalysis in complex solvent environment beyond mean field approximation, developed Python scripts to automatize the process of computation and results analyse, see publication 7 and 8.
- Conducted works to optimize parameters and to improve the accuracy of implicit solvent models including SMD and PCM, developed Shell and Python scripts to systematically optimize parameters using the MNSOL-v2012 data set, proposed "mixed theoretical levels" and "mixed ESF" respectively for SMD and PCM for accurate pKa and redox potential predictions, see publication 5 and 6.
- More details about these projects can be found from my personal website.

MDPI Publisher — Beijing, China

Assistant Editor — July 2018–September 2018

- Managed the review process of the manuscript of two journals *Materials* and *High-throughput* of MDPI publisher.
- Conceived the scope and set up the special issues of the journals.

Sichuan University — Chengdu, China

M.S. in Applied Chemistry (Full scholarship), GPA: 3.72/4.00 — September 2015–June 2018

- Thesis: "Theoretical study on the non-equilibrium solvation effects on the charge-transfer excited state"
- First place in the entrance exam.
- Four publications (see publication 1-4) published in peer-reviewed journals.
- Developed theory for studying non-equilibrium solvation and solvent reorganization in the framework of electrodynamics of continuous media and constrained equilibrium method.
- Implemented the algorithm in codes and apply the theory to the study of electronic excited states.
- More details about these projects can be found from my personal website.
- Main Curriculum: Methods for Mathematical Physics, Numerical Analysis, Computational Chemistry, Bioinformatics

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"
- Minister of outreach department of student union
- Main Curriculum: Fundamentals of Computer, Advanced Mathematics, Advanced Physics, Probability Theory and Mathematical Statistics, Application of Computer in Chemistry, Physical Chemistry, Materials Physics

Publications

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

[9] Mattia Belotti, Xin Lyu, **Longkun Xu**, Peter Halat, Nadim Darwish, Debbie S Silvester, Ching Goh, Ekaterina I Izgorodina, Michelle L Coote, Simone Ciampi. "Experimental Evidence of Long-Lived Electric Fields of Ionic Liquid Bilayers" *J. Am. Chem. Soc.* **2021** 143 (42), 17431–17440. **(First Computational Author)**
[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 7 years (2015-2022) experience with many different aspects of computational chemistry including:
  - Quantum Chemistry: Gaussian, ORCA, Molpro, xtb, MOPAC, COSMOtherm, Q-Chem, GAMESS-US, ADF, etc.)
  - Molecular Dynamics: LAMMPS, TRAVIS, etc.
  - Material Modelling: VASP.
  - Wave Function Analysis: Multiwfn.
  - Molecular Visualization: GaussView, IQmol, CYLview, VMD, PyMol, Avogadro, etc.
  - Neural Network Potential: Attended the first Colombo Academy workshop hosted by Deep Modeling Community, familar with the theory and use of DeepMD-kit and DP-GEN, see credential
  - Others: Openbabel, RDKit
- **Computer Science:**
  - Understand basic Knowledge of data structure, algorithm and database.
  - Coding skills: Shell, Python, R, Julia, Fortran, SQL, etc. My Leetcode profile can be found here.
  - Operating System and Editor: Linux, Vim, VScode, RStudio, Conda, Github and Jupyter.
  - GPU Programming: I attended the *N-Ways GPU Bootcamp* organized by Australia NCI and Nvidia in 2021, which covers the basic knowledge of GPU programming.
  - High Performance Computing: ssh, pbs, CUDA, etc, see credential
  - Web Scraping: Scraper, Scrapy, see credential
- **Machine Learning and Data Science:**
  - Understand the basic theory of machine learning and data science.
  - Have experience with multiple machine learning and deep learning platforms including scikit-learn, JAX, TensorFlow, pytroch, etc.
  - Related Tools: Pandas, NumPy, SciPy, Matplotlib, MySQL, etc.
- **General Math, Physics and Chemistry:**
  - Familiar with linear algebra, calculus, probability and statistics.
  - Familar with quantum mechanics, thermodynamics and electrodynamics
  - Familar with material science, organic chemistry, physical chemistry, analytical chemistry and inorganic chemistry.
- **Scientific Writing:** Be able to write using LaTex, Word, Markdown, etc.

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
- Part-time tutor for students from UCL, University of York, University of Warwick for courses including polymer, computational chemistry, machine learning, R language, research paper writing, etc. 2021–Current