Curriculum Vitae

LIOU, Kai-Hsin

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Education

2016–Present	Ph.D. Chemical Engineering The University of Texas at Austin, USA
2014–2016	M.S. Chemical Engineering National Taiwan University, ROC (Taiwan)
2008–2013	B.S. Chemical Engineering and Electrical Engineering National Taiwan University, ROC (Taiwan)

Research Projects

Current

- Proton transfer in liquid water
- Space-filling curves based real-space grid partitioning methods
- Polynomial filtering eigensolvers for density functional theory based electronic structure calculations

Past

- Computational study of aluminosilicate nanotubes for water desalination
- Computational study of the mechanical and structural properties of aluminosilicate nanotubes

Publications

[1] Timothy Liao, Kai-Hsin Liou, and James R. Chelikowsky. Real-space pseudopotential method for charged Si_nH_m ($n > 1500$) nanocrystals: Screening and vacancy formation. 2022. Submitted.

[2] Kai-Hsin Liou, Ariel Biller, Leeor Kronik, and James R. Chelikowsky. Space-filling curves for real-space electronic structure calculations. *Journal of Chemical Theory and Computation*, 17(7):4039–4048, 2021.

[3] Kai-Hsin Liou, Chao Yang, and James R. Chelikowsky. Scalable implementation of polynomial filtering for density functional theory calculation in parsec. *Computer Physics Communications*, 254:107330, 2020.

[4] Yen-Ru Chen, Kai-Hsin Liou, Dun-Yen Kang, Jiun-Jen Chen, and Li-Chiang Lin. Investigation of the water adsorption properties and structural stability of mil-100(fe) with different anions. *Langmuir*, 34(14):4180–4187, 2018.

[5] Kai-Hsin Liou, Dun-Yen Kang, and Li-Chiang Lin. Investigating the potential of single-walled aluminosilicate nanotubes in water desalination. *ChemPhysChem*, 18(2):179–183, 2017.

[6] Kai-Hsin Liou and Dun-Yen Kang. Defective single-walled aluminosilicate nanotubes: Structural stability and mechanical properties. *ChemNanoMat*, 2(3): 189–195, 2016.

[7] Dun-Yen Kang, Kai-Hsin Liou, and Wei-Lun Chang. Investigating friction as a main source of entropy generation in the expansion of confined gas in a piston-and-cylinder device. *Journal of Chemical Education*, 92(10):1667–1671, 2015.

[8] Kai-Hsin Liou, Nien-Ti Tsou, and Dun-Yen Kang. Relationships among the structural topology, bond strength, and mechanical properties of single-walled aluminosilicate nanotubes. *Nanoscale*, 7(39):16222–16229, 2015.

Presentations

2021	American Physical Society March Meeting, *Space-Filling Curves for Real-Space Pseudopotential Density Functional Theory Calculations*
2020	32nd Electronic Structure Workshop, *A Brief Tutorial on PARSEC*
2019	American Physical Society March Meeting, *Recent Advances in PARSEC for Performing Large-Scale Electronic Structure Calculations in Real Space*
2018	American Physical Society March Meeting, *A Parallel Eigensolver: Using Spectrum Slicing Method to Solve the Kohn–Sham Problem for Large Systems*

Honors and Awards

2016	Dr. Thomas F. Edgar Endowed Graduate Fellowship in Chemical Engineering James R. and Merle Fair Endowed Graduate Fellowship in Chemical Engineering

Professional Experience

2016–Present	Graduate Research Assistant (@ UT Austin)
2018, 2021	Teaching Assistant (@ UT Austin) *Numerical Methods* *Introduction to Computing*
2016	Research Assistant (@ NTU) *Inorganic nanotubes and metal-organic frameworks*
2014–2015	Chemical Engineering Department Software Training Lecturer (@ NTU) *COMSOL Multiphysics*

Skills

Programming Languages

Fortran, Python

Research Tools

COMSOL, LAMMPS, PARSEC, Quantum ESPRESSO

Language

Mandarin Chinese, English, basic Japanese, Taiwanese Hokkien