

Sheng-Lun Liao Ph.D.

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PROFESSIONAL EXPERIENCE and KEY ACHIEVEMENTS

Staff Scientist , Factorial Inc, USA.	Jul 2024 - Present
- Develop thermodynamic methods to predict electrolyte stability. - Built an internal database for electrolytes and trained equivariant graph neural network (GNN) potentials. - Performed machine learning methods for cycle-life prediction. - Applied machine learning to analyze and optimize manufacturing process parameters, improving yield.	
Senior Simulation Engineer , Factorial Inc, USA	May 2023 - Jun 2024
- Parametrized forcefields and optimized electrolyte formulations. - Conducted DFT and MD simulations to predict the electrochemical properties of novel electrolytes.	
Postdoctoral Scholar , Stanford University, USA	Jun 2021 - Apr 2023
- Identified gas production mechanisms in Li-metal batteries via computational modeling (DFT). - Performed molecular dynamics (MD) simulations to study correlated ion transport in electrolytes. - Executed free energy landscape sampling for Li-polysulfide systems.	
Deputy Project Manager , Molecular Science Center, GGA Corp., Taiwan	Aug 2018 - May 2021
- Developed a new method to predict dielectric functions for cross-linking polymers. - Trained machine learning and QSAR models to predict the properties of electrolyte additives.	
Postdoctoral Researcher , National Taiwan University, Taiwan	Mar 2018 - Jul 2018
Unraveled the memory effect of ultrafast electron dynamics in time-dependent DFT.	
Visiting Student Research Collaborator , Princeton University, USA	Sep 2014 - Aug 2015
Solved nonlinear electron dynamics within the framework of time-dependent density functional theory.	
Visiting Researcher , University of Kansas, USA	Sep 2013 - Feb 2014
Optimized attosecond pulse generation through coherent control.	
R&D Alternative Service (compulsory), Taiwan	Sep 2009 - Aug 2012
Developed an efficient algorithm for quantum optimal control theory (100 - 1000 times faster than existing methods).	

SKILLS AND COMPETENCES

Experienced in electrolyte modeling (DFT, MD) and simulation tools such as GROMACS, CP2K, ASE, and Gaussian. Proficient in Python (pandas, NumPy, scikit-learn) and ML frameworks (MACE). Skilled in data analysis and machine learning for manufacturing process optimization, including Bayesian optimization and predictive modeling. Strong background in high-performance computing, parallel computing, version control (Git), and scientific computing.

EDUCATION

Ph.D. in Physics , National Taiwan University	Jan 2018
Dissertation: Development of new quantum optimal control algorithms and the exact optimized effective potential in time-dependent density functional theory.	
M.S. in Physics , National Taiwan University	Jun 2009
Dissertation: Ab initio study of the properties of Bose-Einstein condensates with dipolar interactions in an anisotropic trap.	
B.S. in Physics , National Taiwan University	Jun 2006

FELLOWSHIP

- Leap Program, MOST, Taiwan (2021);
- Graduate Student Study Abroad Program, MOST, Taiwan (2014)

RESEARCH PUBLICATIONS

- [1] Chen, Y. et al., *Hyperconjugation-controlled molecular conformation weakens lithium-ion solvation and stabilizes lithium metal anodes*, Chem. Sci. **15**, 19805 (2024).
- [2] S. C. Kim et al., *Solvation-Property Relationship of Lithium-Sulphur Battery Electrolytes*, Nat. Commun. **15**, 1268 (2024).
- [3] Z. Huang et al., *A Salt-Philic, Solvent-Phobic Interfacial Coating Design for Lithium Metal Electrodes*, Nat. Energy **8**, 577 (2023).
- [4] Y. Lin et al., *Impact of the Fluorination Degree of Ether-Based Electrolyte Solvents on Li-Metal Battery Performance*, J. Mater. Chem. A (2023).

- [5] S. T. Oyakhire, S.-L. Liao, S. B. Shuchi, M. S. Kim, S. C. Kim, Z. Yu, R. A. Vilá, P. E. Rudnicki, Y. Cui, and S. F. Bent, *Proximity Matters: Interfacial Solvation Dictates Solid Electrolyte Interphase Composition*, Nano Lett. **23**, 7524 (2023).
- [6] R.-H. Yang, L.-Y. Chueh, S.-L. Liao, and Y.-T. Pan, *Synthesis of Plasmonic W18O49 Interconnected Nanowire Frameworks with Strong Photo-Enhanced Hydrogen Evolution Reaction Activity*, Mater. Today Sustain. **24**, 100485 (2023).
- [7] C. Carmine, A. Thilakan Puliparambil, C. Tiffany Hsin-Yi, L. Sheng-Lun, K. Kuan Ying, Y. Atsushi, L. Wei Chih, N. Mooi Yoke, and K. Lung Yit, *Tuning of the Electro-Optical Properties of Tetraphenylcyclopentadienone via Substitution of Oxygen with Sterically-Hindered Electron Withdrawing Groups*, Sci Rep-Uk **9**, 12762 (2019).
- [8] S.-L. Liao, T.-S. Ho, H. Rabitz, and S.-I. Chu, *Exact-Exchange Optimized Effective Potential and Memory Effect in Time-Dependent Density Functional Theory*, European Phys J B **91**, 147 (2018).
- [9] S.-L. Liao, T.-S. Ho, H. Rabitz, and S.-I. Chu, *Time-Local Equation for the Exact Optimized Effective Potential in Time-Dependent Density Functional Theory*, Phys Rev Lett **118**, 243001 (2017).
- [10] H. Z. Jooya, P.-C. Li, S.-L. Liao, and S.-I. Chu, *Generation of Isolated Ultra-Short Attosecond Pulses by Coherent Control of the Population of Excited States*, Phys Lett A **380**, 316 (2016).
- [11] S.-L. Liao, T.-S. Ho, H. Rabitz, and S.-I. Chu, *Maximum Attainable Field-Free Molecular Orientation of a Thermal Ensemble with near-Single-Cycle THz Pulses*, Phys Rev A **87**, 013429 (2013).
- [12] S.-L. Liao, T.-S. Ho, S.-I. Chu, and H. Rabitz, *Fast-Kick-off Monotonically Convergent Algorithm for Searching Optimal Control Fields*, Phys Rev A **84**, 031401 (2011).