Tao E. Li

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Professional Appointments

Yale University — **New Haven, CT**
Postdoctoral Associate, Department of Chemistry — *Aug. 2021 –*
Advisor: Sharon Hammes–Schiffer

Education

University of Pennsylvania — **Philadelphia, PA**
Ph.D., Advisor: Joseph E. Subotnik, Department of Chemistry — *June 2016 – July 2021*
Thesis: *Modeling light-matter interactions: From fundamental processes to polariton chemistry*

Uppsala University — **Uppsala, Sweden**
Erasmus Exchange Student — *Aug. 2015 – Jan. 2016*

Nanjing University — **Nanjing, China**
B.S., Kuang Yaming Honors School — *Sept. 2012 – June 2016*
Advisor: Shuhua Li

Awards & Honors

- John G. Miller Fellowship, University of Pennsylvania — May 2020
- VIEST Graduate Fellowship, University of Pennsylvania — Sept. 2019
- Erasmus Mundus Action 2 Scholarship, Uppsala University — Apr. 2015
- First Prize of Elite Program Scholarship, Nanjing University — 2014 – 2015

Publications & Preprints

Peer-reviewed journals

[19] **T. E. Li**, S. Hammes-Schiffer, "QM/MM modeling of vibrational polariton induced energy transfer and chemical dynamics", *J. Am. Chem. Soc.* **2022**, *December*, 10.1021/jacs.2c10170.

[18] **T. E. Li**, Z. Tao, S. Hammes-Schiffer, "Semiclassical real-time nuclear-electronic orbital dynamics for molecular polaritons: Unified theory of electronic and vibrational strong couplings", *J. Chem. Theory Comput.* **2022**, *18*, 2774–2784.

[17] **T. E. Li**, A. Nitzan, S. Hammes-Schiffer, J. E. Subotnik, "Quantum simulations of vibrational strong coupling via path integrals", *J. Phys. Chem. Lett.* **2022**, *13*, 3890–3895.

[16] **T. E. Li**, A. Nitzan, J. E. Subotnik, "Energy-efficient pathway for selectively exciting solute molecules to high vibrational states via solvent vibration-polariton pumping", *Nat. Commun.* **2022**, *13*, 4203.

[15] **T. E. Li**, A. Nitzan, J. E. Subotnik, "Polariton relaxation under vibrational strong coupling: Comparing cavity molecular dynamics simulations against Fermi's golden rule rate", *J. Chem. Phys.* **2022**, *156*, 134106.

[14] **T. E. Li**, B. Cui, J. E. Subotnik, A. Nitzan, "Molecular polaritonics: Chemical dynamics under strong light–matter coupling", *Annu. Rev. Phys. Chem.* **2022**, *73*, 43–71.

[13] **T. E. Li**, A. Nitzan, J. E. Subotnik, "Collective vibrational strong coupling effects on molecular vibrational relaxation and energy transfer: Numerical insights via cavity molecular dynamics simulations", *Angew. Chemie Int. Ed.* **2021**, *60*, 15533–15540.

[12] **T. E. Li**, A. Nitzan, J. E. Subotnik, "Cavity molecular dynamics simulations of vibrational polariton-enhanced molecular nonlinear absorption", *J. Chem. Phys.* **2021**, *154*, 094124.

[11] **T. E. Li**, J. E. Subotnik, A. Nitzan, "Cavity molecular dynamics simulations of liquid water under vibrational ultrastrong coupling", *Proc. Natl. Acad. Sci. USA* **2020**, *117*, 18324–18331.

[10] **T. E. Li**, A. Nitzan, J. E. Subotnik, "On the origin of ground-state vacuum-field catalysis: Equilibrium consideration", *J. Chem. Phys.* **2020**, *152*, 234107.

[9] **T. E. Li**, H.-T. Chen, A. Nitzan, J. E. Subotnik, "Quasiclassical modeling of cavity quantum electrodynamics", *Phys. Rev. A* **2020**, *101*, 033831.

[8] **T. E. Li**, H.-T. Chen, A. Nitzan, J. E. Subotnik, "Understanding the nature of mean-field semiclassical light-matter dynamics: An investigation of energy transfer, electron-electron correlations, external driving, and long-time detailed balance", *Phys. Rev. A* **2019**, *100*, 062509.

[7] H.-T. Chen, **T. E. Li**, A. Nitzan, J. E. Subotnik, "Understanding detailed balance for an electron-radiation system through mixed quantum-classical electrodynamics", *Phys. Rev. A* **2019**, *100*, 010101.

[6] H.-T. Chen, **T. E. Li**, A. Nitzan, J. E. Subotnik, "Predictive semiclassical model for coherent and incoherent emission in the strong field regime: The mollow triplet revisited", *J. Phys. Chem. Lett.* **2019**, *10*, 1331–1336.

[5] **T. E. Li**, H.-T. Chen, J. E. Subotnik, "Comparison of different classical, semiclassical, and quantum treatments of light–matter interactions: Understanding energy conservation", *J. Chem. Theory Comput.* **2019**, *15*, 1957–1973.

[4] H.-T. Chen, **T. E. Li**, M. Sukharev, A. Nitzan, J. E. Subotnik, "Ehrenfest+R dynamics. II. A semiclassical QED framework for Raman scattering", *J. Chem. Phys.* **2019**, *150*, 044103.

[3] H.-T. Chen, **T. E. Li**, M. Sukharev, A. Nitzan, J. E. Subotnik, "Ehrenfest+R dynamics. I. A mixed quantum–classical electrodynamics simulation of spontaneous smission", *J. Chem. Phys.* **2019**, *150*, 044102.

[2] **T. E. Li**, H.-T. Chen, A. Nitzan, M. Sukharev, J. E. Subotnik, "A necessary trade-off for semiclassical electrodynamics: Accurate short-range Coulomb interactions versus the enforcement of causality?", *J. Phys. Chem. Lett.* **2018**, *9*, 5955–5961.

[1] **T. E. Li**, A. Nitzan, M. Sukharev, T. Martinez, H.-T. Chen, J. E. Subotnik, "Mixed quantum–classical electrodynamics: Understanding spontaneous decay and zero-point energy", *Phys. Rev. A* **2018**, *97*, 032105.

Selected Communications

Invited talks

- Rice University, Chemistry Seminar, Houston, TX — Nov. 2022
- ACS Northeast Regional Meeting, Rochester, NY — Oct. 2022

Contributed talks

- ACS Spring Meeting, San Diego, CA — Mar. 2022
- APS March Meeting, virtual — Mar. 2021

Posters

- GRS & GRC Electron Donor-Acceptor Interactions, Newport, RI (**GRS Best Poster Award**) — Aug. 2022
- ACS Fall Meeting, San Diego, CA — Aug. 2019
- GRC Molecular Interactions and Dynamics — July 2018

Academic Services

Independent reviewer

- *J. Chem. Phys.*, *J. Phys. Chem.*, *J. Phys. Chem. Lett.*, *ACS Phys. Chem. Au*

Teaching

Teaching General Chemistry Experiments — Sept. 2016 – May 2017

Software Development

Q-Chem Developer — Sept. 2021 –

Implementing real-time nuclear-electronic orbital density functional theory (RT-NEO-TDDFT) and real-time nuclear-electronic orbital Ehrenfest (RT-NEO-Ehrenfest) dynamics in both free space and optical cavities.

Cavity Molecular Dynamics Simulations Tool Set — Jan. 2020 –

Developing and maintaining an open-source project — cavity molecular dynamics (CavMD) simulations (`https://github.com/TaoELi/cavity-md-ipi`) — for studying novel physical and chemical behaviors of molecular dynamics in the condensed phase under vibrational strong light-matter interactions.

Skills

Programming Languages

- C++, Python, Bash, CUDA

Programming skills

- Machining Learning (Sklearn, Tensor Flow), Parallel Computing (OpenMP, MPI, OpenACC), Linux Cluster Management, 3D Modeling (Blender)