

# Li, Ye (李, 叶)

he/him/his

Last Update: Apr 25, 2026

## INFORMATION & CONTACT

---

I am currently a Ph.D. candidate at [Peking University](#).

Address: College of Chemistry and Molecular Engineering  
Peking University  
Beijing 100871, China

Email: [pkupkupku@pku.edu.cn](mailto:pkupkupku@pku.edu.cn)

## EDUCATION

---

- Ph.D. Student in Physical Chemistry, Peking University 2022-present;  
Advisor: Prof. [Chen Li](#)
- B.S. in Chemistry and Mathematics, Peking University 2018-2022.

## RESEARCH INTERESTS

---

With broad interests spanning theoretical and computational chemistry, my current research focuses on electronic structure theory, specifically developing density functional methods for excited states.

## PUBLICATIONS

---

\*Corresponding Author; †Co-first Authorship.

- Chengeng Sun, **YL**, Chen Li\*, Exact factorization of fermionic many-body excited-state wave functions: Case study of the harmonic problem, *Phys. Rev. A*, Accepted.
- **YL**, Chen Li\*, Efficient prediction of singlet-triplet gaps in delayed fluorescence emitters using Kohn–Sham orbital energies, *J. Phys. Chem. Lett.*, 17(1), 141-148, **2026**. [Link](#)
- Zixuan Wang, **YL**, Chen Li\*, Testing exact-factorization-based density functional approximation on a continuous density model, *J. Chem. Phys.*, 162, 234104, **2025**. [Link](#)
- **YL**, Chen Li\*, Localized orbital scaling correction to linear-response time-dependent density functional approximations, *J. Chem. Theory Comput.*, 21, 11, 5514, **2025**. [Link](#)
- **YL**, Zixuan Wang, Chen Li\*, Understanding molecular geometric phase effects with exact effective force: case study of a model system, *J. Phys.: Condens. Matter*, 36, 465201, **2024**. [Link](#)

## PRESENTATIONS

---

- **Poster presentation:** ‘Localized Orbital Scaling Correction to Linear-response Time-dependent Density Functional Approximations’, *Lennard-Jones Centre-CECAM Meeting 2025: From Electrons to Atoms to Molecules and Materials* ([Link](#)), September 2025, Cambridge, United Kingdom.
- **Poster presentation:** ‘A Preliminary Exploration on the Range-Separation Strategy for Range-Separated Hybrid Functionals’, *11th Triennial Congress of the International Society*

for *Theoretical Chemical Physics (ISTCP 2024)*, October 2024, Qingdao, China.

## TEACHING

---

- Teaching Assistant of *Quantum Chemistry* (Lectured by Prof. [Hong Jiang](#))  
Peking University Spring 2025
- Teaching Assistant of *Structural Chemistry* (Lectured by Prof. [Chen Li](#))  
Peking University Spring 2024

## HONORS & AWARDS

---

As a Graduate Student:

- PKU Pioneer Scholarship 2025
- Industrial Bank Scholarship 2023

As an Undergraduate:

- Excellent Graduate of Peking University 2022
- Tang Youqi-Zhang Lizhu Scholarship 2021
- Peking University Third-Class Scholarship 2019

## LINKS

---

- [My GitHub Repository](#)
- [Chen Li's Research Group at PKU](#)