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# Rui Li

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## EDUCATION

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- Sept 2016 - present*      **Chu Kochen Honors College<sup>1</sup>, Zhejiang University, China**
- Major: Chemistry
  - GPA: 3.85/4.0 (88.34/100)
  - Ranking: **Top 5%** (90 in total)
  - Supervisor: Prof. Zhoupeng Li (<https://person.zju.edu.cn/en/0005009>)  
Prof. Linjun Wang (<https://person.zju.edu.cn/en/linjunwang#766272>)
- Jul 2019 - Dec 2019*      **School of Chemistry, University of Bristol, United Kingdom**
- Summer research project
  - Supervisor: Prof. Fred Manby (<http://www.bris.ac.uk/chemistry/people/fred-r-manby/>)  
Prof. Neil Allan (<http://www.bris.ac.uk/chemistry/people/person/5360>)

## PUBLICATION

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- **R. Li**, Y.J. Ge, L.T. Dou, B.H. Liu and Z.P. Li,  
*Prevention of active-site destruction during the synthesis of high performance non-Pt cathode catalyst for fuel cells*,  
RSC Adv., 2017, 7, 6622
- Issoufou A.M. Ousmane, **R. Li**, C. Wang, G.R. Li, W.L. Cai, B.H. Liu and Z.P. Li,  
*Fabrication of oriented-macroporous-carbon incorporated with  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> for high performance lithium-sulfur battery*,  
Microporous and Mesoporous Materials, 2018, 266, 276-282
- Q.Q. Wang, J.J. Xu, **R. Li**, Z. Lin, B.H. Liu and Z.P. Li,  
*A strategy to deposit nano metals in multi-layer graphene for scalable synthesis of high performance anode materials in lithium ion battery*,  
Journal of Alloys and Compounds, 2018, 731, 739-744

## UNPUBLISHED RESEARCH EXPERIENCE

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- Jul. 2019 - Present*      **entos**
- An *ab initio* molecular dynamics package led by Prof. Fred Manby and Prof. Tom Miller
  - Major Implementation and Contribution:
    - molecular GFN0-xTB method
    - sTDA-xTB method
    - periodic GFN1-xTB method
  - visit <https://www.entos.info> for more details
- Jul. 2019 - Present*      **Cristobalite and Borate Cristobalite**
- Exploration of ultra-flexible low-energy forms of Cristobalite and Borate Cristobalite
  - Supervised by Prof. Neil Allan
  - Relevant reference: <https://doi.org/10.1039/C8FD00052B>
- Oct. 2018 - Present*      **Semi-Classical Moyal Dynamics in multivariate system**
- A semi-classic time-dependent dynamics method based on expectations of observables
  - Supervised by Prof. Linjun Wang
  - Relevant reference: <https://doi.org/10.1063/1.5067005>

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<sup>1</sup>Chu Kochen Honors College admits top 5% students in Zhejiang University.

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## WORK EXPERIENCE

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*Oct. 2016 - Dec. 2016*    **Voluntary tutoring for Yucai Elementary School students**

*Jul. 2018 - Oct. 2018*    **Voluntary tutoring for Xuejun High School students**

*Sept. 2018 - Jan. 2019*    **Teaching Assistant of *General Chemistry***

- in Department of Chemistry, Zhejiang University

## OTHER NOTABLE PROGRAMS

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*Jul. 2019 - Oct. 2019*    **Restricted Hartree-Fock Program**

- Supports all basis sets and arbitrary number of atoms
- The integrations are based on Obara - Saika scheme
- The only dependency is GSL (GNU Scientific Library)
- The results are comparable to the quantum chemistry packages, such as gaussian 16
- Repository: <https://github.com/Walter-Feng/Hartree-Fock>

*Mar. 2019 - Apr. 2019*    **Time Dependent Discrete Variable Representation in 1D**

- Supports input of arbitrary combination of elementary functions
- Based on uniform-grid scheme
- The only dependency is GSL (GNU Scientific Library)
- Repository: <https://github.com/Walter-Feng/SincDVR>

## HONORS AND AWARDS

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*2017*    • Zhejiang Province Government Scholarship

*2017*    • Research and Innovation Award at Zhejiang University

*2017, 2018*    • First-Class Scholarship for Top-notch Students of Basic Disciplines at Zhejiang University

*2018*    • Third-Class Scholarship for Outstanding Merits at Zhejiang University

## ABILITY

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• **Language:** Japanese (native), Chinese (native), English (fluent)

• **Programming Language:** C, C++, Julia, Python, Mathematica

• **Notable softwares:**  $\text{\LaTeX}$ , entos, GAUSSIAN 16, PySCF, CP2K, CASTEP, CRYSTAL17

• **Standardized Tests:** TOEFL (110 = Listening 30 + Speaking 23 + Reading 30 + Writing 27)

GRE General Test ( 324 = Verbal 154 + Quantitative 170, Analytical Writing 3.5)

GRE Chemistry Subject Test (860, 93%)

• **GitHub Account:** <https://github.com/Walter-Feng>