

Jinzhe Zeng

Email: jzzeng@stu.ecnu.edu.cn

Website: <https://cv.njzjz.win>

GitHub: <https://github.com/njzjz>

EDUCATION

School of Chemistry and Molecular Engineering, East China Normal University (ECNU)

B.S. in Chemistry

Member in Talents School of 21st Century, ECNU

Core Courses: Computational Chemistry (**88/100**), Foundation of Algorithm and Programming (**98/100**), College Computer (**95/100**), Chemical Principle (**88/100**), Advanced Mathematics B1 (**95/100**), Advanced Mathematics B2 (**80/100**), etc.

Overall Ranking: **26/77**

PUBLICATIONS

[1] **Zeng, J.**; Cao, L.; Zhang, J. Z. H. ; Chin, C.-H.*; Zhu, T.*; *ReacNetGen: an Automatic Reaction Network Generator for Reactive Molecular Dynamic Simulations* (*submitted*)

[2] **Zeng, J.**; Xu, M.; Zhang, J. Z. H.; Zhu, T.*; *A Machine Learning-Based Approach to Make Datasets from Molecular Dynamics Simulations for Neural Network* (*in preparation*)

[3] Tian, S.; **Zeng, J.**; Liu, X.*; Chen, J.; Zhang, J. Z. H.; Zhu, T.*; *Understanding molecular basis of PI4KIII domain/ligand recognition using computational analysis* (*submitted*)

[4] Cao, L.; **Zeng, J.**; Zhu, T.*; Zhang, J. Z. H.*; *Automated Fragmentation AIMD Calculation for Fuel Combustion* (*in preparation*)

[5] Han, X.-Y.; Chen, Z.-H.; **Zeng, J.-Z.**; Fan, Q.-X.; Fang, Z.-Q.; Shi, G.; Zhang, M.*; *Inorganic-Organic Hybrid Tongue-Mimic for Time-Resolved Luminescent Noninvasive Pattern and Chiral Recognition of Thiols in Biofluids toward Healthcare Monitoring*, *ACS Appl. Mater. Interfaces*, 2018 *10* (37), 31725-31734, DOI: 10.1021/acsami.8b13498 (*published*)

RESEARCH EXPERIENCES

DIRECTION: Theoretical Study on Aviation Fuel Combustion Mechanism

Supervised by Prof. John Zenghui Zhang and Prof. Tong Zhu Sep. 2017 – Present

- Prof. John Zenghui Zhang, Professor at New York University (NYU), ECNU, and NYU Shanghai, Director of NYU-ECNU Center for Computational Chemistry at NYU Shanghai
- Prof. Tong Zhu, Associate Professor of Chemistry at ECNU and NYU-ECNU Center for Computational Chemistry at NYU Shanghai

ReacNetGenerator: ML-Based Reaction Network Generator Mar. 2018 – Jun. 2018

- Developed an automatic generator of reaction network and the analysis report for reactive molecular dynamics simulation based on Hidden Markov Model for filtering noise in the trajectory
- Used SMILES for isomers identifying, force-directed graph drawing algorithms for visualization of reaction network, *multiprocessing* package for parallel computing
- Submitted a paper (Publication [1]), released a software named *ReacNetGenerator* and applied a Computer Software Copyright Registration Certificate

ML-Based Making Datasets for MD and Performing CNN MD May. 2018 – Present

- Made datasets for methane and RP-3 fuel from the trajectory of molecular dynamics simulation based on kMeans and developed a program named *MDDatasetMaker*
- Used *Gaussian16* to calculate energies and forces on MN15/6-31g(d,p) level and trained k-body convolutional neural networks (CNN) with *TensorFlow*

- Performed a CNN MD simulation with modified *LAMMPS* and *kconMD* that we developed
- Wrote a paper (Publication [2]) and released several programs

Automated Fragmentation AIMD Calculation for Fuel Combustion Apr. 2018 – Present

- Used *OpenBabel* for fragmentation and found that fragmentation can speed up AIMD calculation and preserve accuracy
- Developed an automated fragmentation method for AIMD and performed fragmentation AIMD simulations with *Gaussian16* and modified *LAMMPS*
- Wrote a paper (Publication [4]) and released a program named *AIMDFragmentation*

Fragmentation QEq Calculation for Accelerating ReaxFF MD Sep. 2017 – Dec. 2017

- Found fragmentation QEq calculation is accurate but cannot accelerate ReaxFF in *LAMMPS*
- Proved that the time complexity of QEq using a CG algorithm is $O(N)$ so that the fragmentation calculation for QEq is useless

SELECTED PROJECTS

Chemical Tools and Laboratory Safety Management Platform Nov. 2015 – Present

- Developed several software for students in Chemistry, across Windows, Android, iOS, Web and WeChat Mini Program platform, in VB, Java, Object-C, HTML/CSS, PHP, and JavaScript
- Got over 18,000 users, received 8 awards (including 2 national awards) and a Computer Software Copyright Registration Certificate, started a business with it, and received funding from Shanghai College Students Innovation and Entrepreneurship Planning Program

Color: A Bacillus Anthracis Recognizer Jan. 2017 – Jun. 2017

- Developed Android and iOS apps which predict the concentration of 2,6-pyridine dicarboxylic acid according to its color, to recognize Bacillus anthracis and improve people's health
- Won the First Prize in ECNU 25th Da-Xia Cup Extracurricular Academic and Scientific Works Competition

Yi-Qu: A Social Platform of ECNU and SJTU Nov. 2017 – Oct. 2018

- Developed a social platform on WeChat for college students at ECNU and Shanghai Jiao Tong University (SJTU), mainly in JavaScript and CSS
- Received funding from National College Students Innovation and Entrepreneurship Planning Program and won the Second Prize in ECNU 26th Da-Xia Cup Extracurricular Academic and Scientific Works Competition

SELECTED NATIONAL AWARDS

First Prize in Contemporary Undergraduate Mathematical Contest in Modeling Nov. 2018

Second Prize in Chinese College Students Computer Design Contest Aug. 2016 & Aug. 2017

Third Prize in National College Students Mathematics Competition Nov. 2016

TECHNICAL SKILLS

Programming: Python, Shell, C++, Fortran, JavaScript, PHP, HTML, Java, Object-C, Visual Basic

Professional Software: *LAMMPS*, *Gaussian*, *Amber*, *VMD*, *OpenBabel*, *RDkit*, *VASP*, *DeePMD*

Certificate: Shanghai College Computer Rank Examination – Python (Level 2): **100/100** (Full Score)

Professional Python Packages: *TensorFlow*, *NumPy*, *SciPy*, *scikit-learn*, *matplotlib*, *NetworkX*