Yaoyukun Jiang

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EDUCATION

Rutgers University, Department of Chemistry and Chemical Biology — Piscataway, NJ
Ph.D. in Chemistry — 01/2021

Jilin University, College of Chemistry — Changchun, China
B.E. in Polymer Materials and Engineering — 07/2015

Peking University, College of Chemistry and Molecular Engineering — Beijing, China
Exchange Student in Applied Chemistry — 09/2013 – 06/2014

TECHNICAL SKILLS

- Computational chemistry software: Gaussian, TeraChem, AMBER, GROMACS
- Programing: FORTRAN, Python, shell scripting
- TRAVIS, Curves+, Grace, Origin, VMD, PyMOL, LaTeX, EndNote, ChemDraw, Mathematica

RESEARCH EXPERIENCE

Ph.D. with Prof. Lu Wang — 09/2015 – present
Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ

Project 1: Establishing theoretical schemes that accurately and efficiently predict the spectral features of nucleic acids

- Introduced the first theoretical maps to correctly predict the vibrational frequencies of nucleobase carbonyls
- Developed the first models to accurately describe the vibrational couplings of nucleobases
- Performed the GPU-accelerated quantum frequency analyses of nucleic acid water clusters
- Predicted the theoretical IR spectra of nucleic acids correctly using line shape theory
- Illustrated the sensitivity of the coupling to the stacking and pairing of nucleobases
- Validated the necessity of choosing the transition charge model over the transition dipole coupling model

Project 2: Modeling the Structure and Infrared Spectra of Omega-3 Fatty Acid Esters

- Investigated the conformation and packing of eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) esters
- Demonstrated the slow translational and rotational dynamics of EPA and DHA esters
- Calculated the IR spectra of EPA and DHA esters in the inhomogeneous limit
- Revealed the competition mechanism between the inter and intramolecular electrostatic interactions to modulate the frequencies of the ester carbonyl groups

Undergraduate Researcher with Prof. Shimei Jiang and Prof. Wenke Zhang — 05/2012 – 05/2015
State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China

- Synthesized the cyanostilbene derivatives and studied their aggregation-induced emission properties
- Modified the probe tip of atomic force microscope through the Biotin-Streptavidin and Au-S interaction

PUBLICATIONS

- Meng, W.*; **Jiang, Y**.*; Rothschild, D.; Lipke, M.; Hall, G.; Wang, L. Modeling the Structure and Infrared Spectra of Omega-3 Fatty Acid Esters. *J. Chem. Phys.* **2020**, *153*, 035101 (*Equal contribution)
- **Jiang, Y**.; Wang, L. Modeling the Vibrational Couplings of Nucleobases. *J. Chem. Phys.* **2020**, *152*, 084114
- **Jiang, Y**.; Wang, L. Development of Vibrational Frequency Maps for Nucleobases. *J. Phys. Chem. B.* **2019**, *123*, 5791-5804
- Liang, C.; Bu, W.; Li, C.; Men, G.; Deng, M.; **Jiangyao, Y**.; Sun, H.; Jiang, S. A Highly Selective Fluorescent Sensor for Al^{3+} and the Use of the Resulting Complex as a Secondary Sensor for PPi in Aqueous Media: Its Applicability in Live Cell Imaging. *Dalton T.* **2015**, *44*, 11352-11359

PRESENTATIONS

- Lightning Talk & Poster: "Modeling the Vibrational Frequency and Coupling for Nucleobases" at the Virtual Conference on Theoretical Chemistry, July 27 – 29, **2020**
- Poster: "Theoretical Modeling of the Vibrational Spectra of Nucleobases" at the 258th ACS National Meeting & Exposition, San Diego, CA, August 25 – 29, **2019** (Physical chemistry division)
- Poster: "Theoretical Modeling of the Vibrational Spectra of Nucleic Acids" at the 256th ACS National Meeting & Exposition, Boston, MA, August 19 – 23, **2018** (Sci-Mix & computational chemistry division)

TEACHING EXPERIENCE

Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ   09/2016 – 12/2019

- Mentored junior graduate students and undergraduate students on related computational skills such as software usage and coding
- Tutored an undergraduate student for general and organic chemistry each week
- Supervised and instructed undergraduate students in the Organic Laboratory (Chem 311) in techniques of organic chemistry experiments each week.

HORNORS AND AWARDS

Reid Award for Exceptional Performance in Research (highest honor in the department), Rutgers University	2020
Graduate Fellowship, Rutgers University	2018, 2017, 2015
Conference Travel Fund, Rutgers University	2018
Teaching Assistant and Graduate Assistant Professional Development Fund, Rutgers University	2018
J. Livingston Rutgers Morgan Award, Rutgers University	2015
Scholarship of Dalian Institute of Chemical Physics, Jilin University	2013
First Prize of Excellent Undergraduate Scholarship, Jilin University	2013, 2012
National Scholarship, Ministry of Education of the People's Republic of China	2012