

# Lianjun (Ellie) Zheng

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## EDUCATION

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*Duke University, Durham, NC*

<b>Ph.D., Computational Chemistry</b>	expected 05/2019
<b>Certificate in College Teaching</b>	expected 05/2019
<b>Graduate Certificate in Nanoscience</b>	expected 05/2019

*Peking University, Beijing, China*

<b>B.S., Chemistry</b>	06/2013
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## RESEARCH EXPERIENCE

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*Department of Chemistry, Duke University, Durham, NC*

### **Graduate Research Assistant, Adviser: Dr. David N. Beratan**

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|---|----------------|
| ○ Introducing extra bias to the compounds filtering step in the property-optimizing ACSESS algorithm, a framework to develop diversity oriented molecular libraries, for rational design of chromophores. | 2018 – present |
| ○ Investigating the mechanism of charge transports in self-assembled cyclic peptide nanotubes.  | 2017 – present |
| ○ Designed linear light absorbers based on the quantum-optical analogy.   | 2015 – 2017    |
| ○ Explored the physics underpinning the orders of magnitude enhancement of polyene light absorption induced by electrostatic fields.  | 2015 – 2017    |
| ○ Investigated the oscillator strength distributions in quantum models and in molecules to rationalize the low absorption in the UV/Vis spectral region in molecules.                                     | 2014 – 2015    |

*College of Chemistry and Molecular Engineering, Peking University, Beijing, China*

### **Undergraduate Research Assistant, Adviser: Dr. Kai Wu**

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|---|-------------|
| ○ Synthesized highly ordered Sn <sub>2</sub> O <sub>3</sub> nanowire and Ta <sub>2</sub> O <sub>5</sub> nanotube arrays via template-assisted CVD and anodic oxidation. | 2012 – 2013 |
| ○ Improved a template-assisted method to synthesizing single crystalline nanowire arrays of high-aspect-ratio.  | 2011 – 2012 |

## TEACHING EXPERIENCE

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*Duke Kunshan University, Kunshan, Jiangsu, China*

**Teaching Assistant**, to be determined 09/2018 – 12/2018

*Department of Chemistry, Duke University, Durham, NC*

**Teaching Assistant**, Biophysical Chemistry 01/2018 – 05/2018

**Course Development Assistant**, Biophysical Chemistry 09/2017 – 12/2017

**Teaching Assistant** (peer reviewed), Biophysical Chemistry 01/2017 – 05/2017

**Undergraduate Student Supervisor**, Research Independent Study 09/2016 – 05/2017

**Teaching Assistant**, Modern Applications of Chemical Principles – Lab 01/2014 – 04/2014

**Teaching Assistant**, Core Concepts in Chemistry – Lab 09/2013 – 12/2013

## COMPUTER SCIENCE EXPERIENCE

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**WheePin – A Web Application** 06/2018 – present

Developing a web application that users could make posts that pinned to their current locations, using the Java Spring framework. A group project.

**PhilistineHome – A Small Internet Forum** 05/2018 – 06/2018

Built a small Internet forum where users could share their thoughts on anime, music, and life. Used by my friends and families (~10 users).

**Athena – An iOS App** 10/2017 – 12/2017

Project for the *Mobile App Development* course at Duke (**Grade: A+**)

Wrote an iOS app called “Athena” using Swift, which helps the users find sport players with matched skill levels and schedule games.

Available at the Duke App Store.

**“Baby” Command Shell using C++** 10/2016 – 12/2016

Project for the *Programming, Data structure & Algorithms in C++* course at Duke (**Grade: A+**)

Wrote a C++ program package that has the basic Linux shell functions, free of warnings and memory leak, coded defensively.

**GPU Optimization for Stencil-Based Hemodynamics Simulation** 10/2015 – 12/2015

Group project for the *Parallel Computing* course, collaborated with Dr. Amanda Randles’s lab at Duke University (**Grade: A+**)

Exploited and analyzed parallelism in the stencil-based computational model of blood flow simulation using GPU. Achieved a speedup up to 20.

## TECHNICAL SKILLS

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### Computational Chemistry

NWChem, Gaussian (quantum mechanics)  
NAMD, VMD (molecular dynamics)  
Mathematica, Origin, Latex

### Data Science

Machine learning  
(using Python pandas and scikit-learn)

### Materials Science

Chemical vapor deposition  
Scanning electron microscopy  
X-Ray diffraction

### Programming

C/C++, Python, Swift, Unix shell script  
HTML/CSS, iOS app development  
Git

### Parallel Computing

OpenMP, CilkPlus, TBB, MPI, CUDA  
(based on C/C++)

### Languages

Chinese (native)  
English (full professional proficiency)  
Japanese (limited working proficiency)

## AWARDS

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*Duke Kunshan University, Jiangsu, China*

**Graduate Teaching Fellowship Award**  
(2018)

*Duke University, Durham, NC*

**Graduate Travel Award** (2016)

**GPNano Fellowship** (2014)

*Peking University, Beijing, China*

**Honors Students** (2012)

**Pan Gu Scholarship** (2012)

**Academic Excellence Award** (2011)

**Wusi Scholarship** (2010&2011)

**Excellent Freshmen** (2009)

## PUBLICATIONS & CONFERENCES

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**L. Zheng**, N. F. Polizzi, A. R. Dave, A. Migliore, D. N. Beratan. Where Is the Electronic Oscillator Strength? Mapping Oscillator Strength across Molecular Absorption Spectra. *J. Phys. Chem. A.*, **2016**, 120 (11), 1933.

J. Shang, B. Huang, J. Yu, Y. Wang, H. Song, J. Dai, C. Chen, **L. Zheng**, K. Wu, et al. Morphological Evolution of In<sub>2</sub>O<sub>3</sub> Crystallites by Metallothermal Reaction Growth: A Unified Elucidation. *J. Clust Sci.*, **2017**, 28 (5), 2733.

**L. Zheng**, A. Migliore, D. N. Beratan. Significant Enhancement of Polyene Light Absorption Induced by Electrostatic Fields. In preparation.

**L. Zheng**, S. Roy, O. Silberbush, A. Migliore, N. Ashkenasy, D. N. Beratan. The Enormous Influence of Side Chain Flexibility on Intermolecular Proton Transfer in Self-Assembled Peptide Nanotubes. In preparation.

- L. Zheng**, A. Migliore, D. N. Beratan. Significant Enhancement of Polyene Light Absorption Induced by Electrostatic Fields. Presented at the third Annual Duke Chemistry Graduate Research Symposium, *Duke University, Durham, NC* (September, 2017).
- L. Zheng**, A. Migliore, D. N. Beratan. Significant Enhancement of Polyene Light Absorption Induced by Electrostatic Fields. Presented at the American Conference on Theoretical Chemistry, *Boston University, Boston, MA* (July, 2017).
- L. Zheng**, N. F. Polizzi, A. R. Dave, A. Migliore, D. N. Beratan. Where Is the Electronic Oscillator Strength in Molecules? Toward Strategies for Oscillator Strength Focusing. Presented at the Gordon Research Conferences: Solar Energy Conversion, *Hong Kong University of Science and Technology, Hong Kong, China* (July, 2016).
- L. Zheng**, N. F. Polizzi, A. R. Dave, A. Migliore, D. N. Beratan. Investigations of Oscillator Strength Focusing. Presented at the annual meeting of the Southeast Theoretical Chemistry Association, *University of Central Florida, Orlando, FL* (May, 2015)