

“The people who are crazy enough to think they can change the world are the ones who do.”

## Education

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### Louisiana State University

PH.D. IN CHEMISTRY

- Under the supervision of Prof. Revati Kumar

*Baton Rouge, U.S.*

*Aug. 2014 - PRESENT*

### Louisiana State University

M.S. IN COMPUTER SCIENCE

*Baton Rouge, U.S.*

*Aug. 2017 - PRESENT*

### Nicholls State University

B.S. IN CHEMISTRY

- GPA: 3.78/4.0, President's List from 2012 to 2014

*Thibodaux, U.S.*

*May 2014*

## Skills

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**Programming** Python, C/C++, bash, tcl, Java, JavaScript, Go, LaTeX, Scheme

**Software** LAMMPS, Amber, Gaussian, Gromacs, NWChem, VMD, Pymol, Matplotlib, gnuplot, docker, git

**Languages** Chinese, English

## Professional Experience

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### Prof. Revati Kumar's Research Lab

GRADUATE RESEARCH ASSISTANT

- Administer theoretical studies on molecular modeling.
- Perform computational simulations to study the polymer chain, micelle formation as well as aggregation in aqueous solutions.
- Develop new force field for varying systems.

*Baton Rouge, U.S.*

*Nov. 2014 - PRESENT*

### Pacific Northwest National Laboratory

STUDENT VISITOR OF DR. MARCEL BAER'S RESEARCH LAB

- learned about QM/MM methods, specifically for peptoids and certain specific side chains.

*Richland, U.S.*

*Oct. 22nd 2017 - Oct. 28th 2017*

### Virginia Tech

PARTICIPANT AT THIRD ANNUAL SOFTWARE SUMMER SCHOOL

- Covered a range of software design and optimization topics, including software development, computer architectures, numerical libraries, parallel computing, and GPU/accelerator algorithms.

*Blacksburg, U.S.*

*Jun. 22nd 2015 - Jul. 1st 2015*

### Undergraduate Research, Chemistry Lab(Prof. Darcey Wayment)

RESEARCH ASSISTANT FOR <LOW-COST TECHNOLOGY FOR MICROFLUIDIC APPLICATIONS>

- Designed a microfluidic chip that will be able to apply into analytical experiments.
- Fabricated the microfluidic chip with laser printer and transparency films independently.

*Thibodaux, U.S.*

*Aug. 2013 - May. 2014*

### Undergraduate Research, Chemistry Lab(Prof. Vincent Sichula)

RESEARCH ASSISTANT FOR <SYNTHESIS OF ORGANIC DYE-SENSITIZERS FOR SOLAR CELLS>

- Worked on the synthesis experiments of organic dye-sensitizer.
- Conducted the UV-vis absorption measurements and cyclic voltammetric measurements of the synthesized intermediate products.
- Performed Column Chromatography to purify compounds.

*Thibodaux, U.S.*

*Aug. 2012 - July. 2013*

## Honors & Awards

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### DOMESTIC

- 2018 **Advancing Science Conference Grant**, The 45th Annual NOBCChE Conference *Orlando, U.S.*
- 2014 **Outstanding Graduate Award**, Nicholls State University *Thibodaux, U.S.*
- 2014 **SGA International Student Scholarship**, Nicholls State University *Thibodaux, U.S.*
- 2012 **President's List**, Nicholls State University *Thibodaux, U.S.*

### INTERNATIONAL

- 2011 **Excellent Student Scholarship**, Chongqing University of Posts and Telecommunications *Chongqing, China*
- 2011 **First place**, Mathematical Modeling Contest *Chongqing, China*
- 2010 **Excellent Student Leadership Award**, Chongqing University of Posts and Telecommunications *Chongqing, China*
- 2010 **Honor Student**, Chongqing University of Posts and Telecommunications *Chongqing, China*

## Presentations

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### 1st North West Theoretical Chemistry Conference (NWTCC)

*Richland, U.S.*

#### ORAL PRESENTATION

*Oct. 2017*

- Development of a coarse-grained model of polypeptoids

### 253rd ACS National Meeting

*San Francisco, U.S.*

#### POSTER PRESENTATION

*Apr. 2017*

- Can zwitterionic cyclic polymers show aggregation in solution?

### 253rd ACS national Meeting

*San Francisco, U.S.*

#### POSTER PRESENTATION

*Apr. 2017*

- Development of a coarse-grained model of polypeptoids for studying self-assembly in solution

### APS March Meeting

*New Orleans, U.S.*

#### POSTER PRESENTATION

*Mar. 2017*

- Development of a coarse-grained model of polypeptoids for studying self-assembly in solution

### 3rd Annual APTEC November Meeting

*New Orleans, U.S.*

#### POSTER PRESENTATION

*Nov. 2015*

- A molecular dynamics study of cyclic and linear polypeptoids

## Publications

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### JOURNAL ARTICLES

The effect of electrostatic interactions on self-assembled structures of sequence-defined peptoid block copolymers

Pu Du, Revati Kumar

*ACS Macro Lett.* (2018). Manuscript in Preparation, 2018

Towards a coarse-grained model of the peptoid backbone: the case of N,N-dimethylacetamide

Pu Du, Steven W. Rick, Revati Kumar

*Phys. Chem. Chem. Phys.* (2018). Accepted Manuscript, 2018

High concentrated glyme-based electrolytes with unusually high conductivities for sodium batteries

Susith R. Galle Kankanamge, Ke Li, Kristen D. Fulter, Pu Du, Ryan Jorn, Revati Kumar, Daniel Kuroda

*ACS Appl. Energy Mater.* (2018). Under Review, 2018

Enantioselective functionalization of enamides at the beta-carbon center with indoles

Mirza Saputra, Binod Nepal, Nitin Dange, Pu Du, Frank Fronczek, Revati Kumar, Rendy Kartika

*Angew. Chem.* (2018). Accepted Manuscript, 2018

Aggregation of cyclic polypeptoids bearing zwitterionic end-groups with attractive dipole-dipole and solvophobic interactions: a study by small-angle neutron scattering and molecular dynamics simulation

Pu Du, Ang Li, Xin Li, Yueheng Zhang, Changwoo Do, Lilin He, Steven W. Rick, Vijay T. John, Revati Kumar, Donghui Zhang

*Phys. Chem. Chem. Phys.* 19 (22 2017) pp. 14388–14400. The Royal Society of Chemistry, 2017