

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

Education

Louisiana State University

PH.D. IN CHEMISTRY

- Under the supervision of Prof. Revati Kumar

Louisiana, U.S.

Aug. 2014 - PRESENT

Louisiana State University

M.S. IN COMPUTER SCIENCE

- Under the supervision of Prof. Qingyang Wang

Louisiana, U.S.

Aug. 2017 - PRESENT

Nicholls State University

B.S. IN CHEMISTRY

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

Louisiana, U.S.

May 2014

Skills

Programming Python, C/C++, Scheme, Java, JavaScript, LaTeX

Software LAMMPS, Tensorflow, Amber, Gaussian, NWChem, Matplotlib

Languages Chinese, English

Professional Experience

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

DOMESTIC

- 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

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

JOURNAL ARTICLES

The effect of electrostatic interactions on self-assembled structures of sequence-defiend 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). Under Review, 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

Enantioconvergent functionalization of enamides at the beta-position with indoles under chiral Brønsted acid catalysis

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

J. Am. Chem. Soc. (2018). Under Review, 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