

## CONTACT INFORMATION

### **Tingting Han**

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## EDUCATION

### ***Doctor of Philosophy, Physical Chemistry***

Clemson University, Clemson, SC

Date of Graduation: August, 2016

Dissertation – “Molecular mechanics study of protein folding and protein-ligand binding”

### ***Bachelor of Science, Applied Chemistry***

Xi'an Jiaotong University, Xi'an, China

Date of Graduation: July, 2008

## EMPLOYMENT

### **Assistant Professor of Chemistry**

Southern Wesleyan University

2016 - Present

### **Data Analyst Internship**

*Risk Engineering & System Analytics Center at Clemson University*

January - May 2016

### **Teaching Assistant & Research Assistant**

*Clemson University*

2011-2015

## EXPERIENCE

### **Southern Wesleyan University**

*Assistant Professor of Chemistry*

2016-Present

CHEM 1004 & 100L General Chemistry I & Laboratory

CHEM 1054 & 105L General Chemistry II & Laboratory

CHEM 2504 & 250L Organic Chemistry I & Laboratory

CHEM 2514 & 251L Organic Chemistry II & Laboratory

CHEM 3404 & 340L Inorganic Analysis & Laboratory

CHEM 3414 & 341L Organic Analysis & Laboratory

### **Clemson University**

*Teaching Assistant*

2013-2015

CHEM 101L General Chemistry I Laboratory

CHEM 102L General Chemistry II Laboratory

## Research Experience

*Department of Chemistry, Clemson University*

2012-2016

- Predicting effect of mutations on protein folding free energies  
In order to better understand the relationship between protein structure and function, it is necessary to accurately predict protein stability changes upon single mutation. A computational method, applying molecular dynamics simulation, was developed to calculate the effect of mutations on protein stability. The importance of conformational sampling and electrostatics in protein stability were also addressed in this study.
- Effect of accumulated mutations in plasmodium falciparum (*pf*) dihydrofolate reductase (DHFR) drug resistance  
DHFR in *pf* is the target for antimalarial drugs. Pyrimethamin (Pyr) is one of antimalarial drugs. However, during the course of Pyr treatment, mutations emerge and lead to antimalarial resistance. To gain more insight into the drug resistance mechanisms, molecular dynamics simulations were applied to study the wild type and mutants *pf*DHFR-Pyr complexes. The results indicated that antimalarial resistance is related to significant conformation and flexibility changes upon mutations in *pf*DHFR.
- Effect of accumulated mutations on plasmodium falciparum dihydrofolate reductase (*pf*DHFR) activity  
The goal of this study was to gain more insight into the catalytic mechanism, and changes of activation energy upon mutations in *pf*DHFR. The transition state analogue method and molecular dynamic simulations were applied to investigate the activity properties. This study found that the hydride transfer geometry in the initial state is important in the enzyme catalysis.

*Department of Material Science & Engineering, Clemson University*

2010-2011

- Surface modifications of biochip substrates  
The failure in attachment between hydrogel and the inorganic surface may lead to the failure of the biosensor. In order to improve the attachment and adhesion of bioactive hydrogels to glass substrates, surface modifications with different chemistries were studied. The principle of hydrogen bonding and the addition polymerization were utilized to guide the surface modification.

*Department of Science, Xi'an Jiaotong University, China*

2008-2010

- Modification of polyurethane  
EHTPB-based polyurethane was developed to replace HTPB-based polyurethane for the benefit of mechanical properties and life span. In this project, I improved the polyurethane curing technique to improve its mechanical properties, and developed the life span predicting model.

## PUBLICATIONS

Jia, Zhe., Ackroyd, C., Han, T., Agrawal, V., Liu, Y., Christensen, K., Dominy, B., Effects from Metal Ion in Tumor Endothelial Marker 8 and Anthrax Protective Antigen: BioLayer Interferometry Experiment and Molecular Dynamics Simulation Study, *Journal of Computational Chemistry* 2017, 38(15):1183-1190

- Li, X., Han, T., Y. Zhang, Hu, J., Zheng, Y., Study on characterization method of Stacking volume resistance of conductive fillers, *Precious Metals* 2010, 31(4):1-6.
- Zhang, Y., Gao, G., Han, T., Zheng, Y., Study on grafting reaction of Ferrocenecarboxylic acid with epoxidized hydroxyl-terminated polybutadiene, *Chemical Propellants& Polymer Materials* 2011,1:78-80.

## PRESENTATIONS

- Tingting Han, Vibhor Agrawal, Yinling Liu, Zhe Jia, and Brian N. Dominy , “Effect of accumulation of mutations in plasmodius falciparum dihydrofolate reductase activity” 250<sup>th</sup> American Chemical Society Meeting, Boston, MA, Aug. 16-20, 2015
- Tingting Han, Brian Dominy, “Perturbation of dynamic properties through mutations in plasmodium falciparum dihydrofolate reductase” Computational Biophysics to Systems Biology Conference, Oklahoma City, OK, May, 17-19, 2015.
- Tingting Han, Brian Dominy, “A study of accumulation of mutations in plasmodius falciparum dihydrofolate reductase”. Southeast Annual Enzyme Conference, Atlanta, GA, Apr. 11, 2015.

## PROFESSIONAL ORGANIZATIONS

American Chemical Society, Member

2018 - Present

## COMPUTER SKILLS

Learning management system including Blackboard, Canvas  
 Programing skills in Matlab, Python, R, Shell Scripts, SAS  
 Molecular dynamics simulation software including CHARMM, NAMD, VMD

## HONORS AND AWARDS

- **Award of Professional Enrichment Grant (PEG)** at Clemson University 2015
- **Fellowship** in “From Computational Biophysics to Systems Biology” Conference 2015
- **Contributed Talk Award** in “From Computational Biophysics to Systems Biology Conference” 2015
- **First Place** for the College of Engineering & Science at the 2014 Clemson Graduate Research and Discovery Symposium 2014
- **Outstanding Graduate Award** of Xi’an Jiaotong University 2008
- **Outstanding Student Award** of Xi’an Jiaotong University 2007
- **National Inspirational Scholarship** 2007
- **National Scholarship** 2006
- **Outstanding Student Leader Award** of Xi’an Jiaotong University 2006