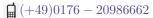
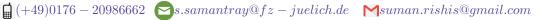


# SUMAN SAMANTRAY

IBI-7: Structural Biochemistry, FZ Jülich, Wilhelm-Johnen-Straße, 52425 Jülich, Germany







♥ @samantray\_1990





## Research Interests

Amyloid aggregation, Interfacial phenomena, Molecular simulation, Computational Chemistry, Machine Learning, Drug discovery, Graph convolutional neural networks

#### EDUCATION

■ IBI-7: Structural Biochemistry, FZ Jülich, Jülich, Germany / AICES fellow, RWTH Aachen University, Aachen, Germany Doctor of Philosophy (Dr. rer. nat.) in Computational Biochemistry

Aug 2018 - present

- > Dissertation: Simulation of Amyloid Aggregation under in vivo Conditions Supervisor: Prof. (Dr.) Birgit Strodel
- State University of New York, Buffalo, USA Master of Engineering (M.Eng) in Chemical Engineering

Aug 2013 - Aug 2015

> Dissertation: Calculation of Saturation and Interfacial properties of model Carbon Dioxide-Water system using Monte Carlo Simulation.

Supervisor: Prof. (Dr.) Jeffrey R. Errington

■ Indira Gandhi Institute of Technology, Odisha, India Bachelor of Technology (B. Tech) in Chemical Engineering Aug 2009 -Jun 2013

> Dissertation: Synthesis of activated carbon from Jackfruit peel waste and Coconut husk for Purification of water.

Supervisor: Prof. (Dr.) Satyabrata Mohanta

### RESEARCH EXPERIENCE

■ Ph.D. Researcher

IBI-7: Structural Biochemistry, FZ Jülich, Germany

Aug 2018-Present Prof. (Dr.) Birgit Strodel

- > Determination of molecular mechanics parameters and building kinetic transition models to elucidate the amyloid-β aggregation pathways.
- > Identification of bio-mimetic molecules inhibiting amyloid-β aggregation.
- > Development of simulation methods for studying amyloid aggregation under the influence of glycosaminoglycans.
- > Co-organiser of hands-on workshop on Molecular Dynamics Simulations of Proteins at IHRS BioSoft.
- > Co-supervision of Strodel group online code databases on GitHub.
- ➤ Maintenance of Strodel group computing clusters and cloud storage services.
- > Co-mentoring of HiWi and M.Sc. students in the Strodel group.
- College of Science postgraduate fellow School of Chemistry, NUI Galway, Ireland

Jan 2017-Jul 2018 Prof. (Dr.) David L. Cheung

- > Using molecular simulation to understand the behaviour of Intrinsically disordered/ Amyloidogenic proteins at air-water interface (AWI).
- > Using the replica exchange and metadynamics simulations to investigate protein structures at liquid interfaces.

#### Research Associate

Oct 2016-Dec 2016

Dept. of Industrial Design, NIT Rourkela, India

Prof. (Dr.) Dibya Prakash Jena

- > Worked in the Industrial Acoustics lab to identify a benchmark acoustic cloaking device.
- > Built an impedance tube with an attached cylindrical Helmholtz resonator to evaluate net acoustic transmission loss using transfer matrix method.

## ■ Graduate Research Student

SUNY Buffalo, NY, USA

Sep 2013-Sept 2015

Prof. (Dr.) Jeffrey R. Errington

- > Applied Grand Canonical Monte Carlo simulation method to compute vapor-liquid coexistence properties of carbon dioxide and water fluid mixture.
- > Used free energy-based approach to determine interfacial properties of the binary fluid mixture including activity fraction expanded ensemble technique on atomistic silica-like surface.
- > Developed algorithms in python to analyze and interpret data from GCMC simulation.

#### Professional Experience

#### ■ Computing Assistant

Information Solutions and Services, NUI Galway, Ireland

Aug 2017–Jul 2018

Mr. Peter Crampton

- > Responsible for the management, development, physical upkeep and maintenance of the ISS and departmental PC suites across campus.
- > Assist the Desktop Services, Provisioning and Support Manager with the provision of this service, ensuring that PC suites are fully operational in all respects.

#### ■ Senior Application Developer

Oct 2015-Sept 2016

Digital products and interactive media (DPIM) III, NBC Universal, NY, USA

Mr. Wen Qu, Mrs. Dana Fleur

- ➤ Lead a team of 3 Dev's and 2 QA's to develop MPS mobile SDK and built a Test App to displays ads fetch SDK users (NBC native apps) and configure it for vendors purposes during **Rio Olympics 2016**.
- > Developed the NBCUView and recently implemented Apple Push Notification Service. Documented the app architecture including identification of the service end points.

#### TEACHING EXPERIENCE

## ■ Teaching Instructor

School of Chemistry, NUI Galway, Ireland

Oct 2017–Apr 2018

Prof. (Dr.) David L. Cheung

- > Teaching Assistant for Computational Drug Design and Drug Discovery laboratory, Spring 2018
- > Teaching Assistant for Physical Chemistry laboratory, Fall 2017

## ■ Teaching Instructor

Centre for Talented Youth, Dublin City University, Ireland

Jul 2017-Aug 2017

Dr. Eleanor Healion

> Demonstration and lecturing on chemistry experiments to primary and secondary school students.

# **PUBLICATIONS**

- [8] Effect of glycosaminoglycans on the dimerisation pathways of amyloid-βpeptide, S. Samantray, B. Strodel, (In preparation), Journal of Physical Chemistry B
- [7] Elucidating the structure of glycosaminoglycans under different physiological conditions, S. Samantray, O.O. Olubiyi, B. Strodel, (In preparation), Biomolecules
- [6] Thermodynamics and kinetics of the amyloid-βpeptide revealed by Markov state models based on MD data in agreement with experiment, A. Paul, S. Samantray, M. Anteghini, B. Strodel, (In Review), Chemical Science
- [5] Molecular dynamics simulations of protein aggregation: protocols for simulation setup and analysis with Markov state models and transition networks, S. Samantray, W. Schumann, A.-M. Illig, M.-C. Pacheco, A. Paul, B. Barz, B. Strodel, (In Press), Methods in Molecular Biology (Springer)
- [4] Effect of the Air-Water Interface on the Conformation of Amyloid Beta, S. Samantray, D.L. Cheung, (Just accepted), Biointerphases
- [3] Different force fields give rise to different amyloid aggregation pathways in molecular dynamics simulations, S. Samantray, F. Yin, B. Kav, B. Strodel, (Just accepted), Journal of Chemical Information and modelling
- [2] β-Turn mimetic synthetic peptides as amyloid-β aggregation inhibitors, S. Deike, S. Rothemund, B. Voigt, S. Samantray, B. Strodel, W.H. Binder, *Bioorganic Chemistry*, 101, 104012 (2020)
- [1] Molecular dynamics simulation of protein biosurfactants, D.L. Cheung, S. Samantray, Colloids Interfaces, 2 (3), 39 (2018)

# Conference Presentations

[1] "Behaviour of intrinsically disordered proteins at liquid interfaces: insights from molecular simulations", Nanoscale Simulators Meeting of Ireland, University of Limerick, Ireland (May 2018).

## POSTER PRESENTATIONS

- [8] "Simulation Studies of Amyloid-β Peptide and its Interactions with Membranes and Glycosaminoglycans", 5<sup>th</sup> Ulm Meeting on "Biophysics of Amyloid Formation", Ulm University, Germany (Feb 2020)
- [7] "Role of physiological environments in the folding of Amyloid-β: Insights from molecular simulations", 3<sup>rd</sup> Düsseldorf-Juelich Symposium on Neurodegenerative Diseases, Düsseldorf, Germany (Nov 2019).
- [6] "Structure and Assembly Dynamics of Amyloidogenic Peptides in Aqueous Solution and at Liquid Interfaces", Computer Simulation and Theory of Macromolecules, Huenfeld, Germany (Mar 2019).
- [5] "Role of physiological environments in the folding mechanism of intrinsically disordered proteins", Biennial Meeting of the German Biophysical Society, Düsseldorf, Germany (Sep 2018).
- [4] "Behaviour of intrinsically disordered proteins at liquid interfaces: Insights from molecular simulations", 70<sup>th</sup> Irish Universities Chemistry Research Colloquium, Queen's University Belfast, UK (Jun 2018).
- [3] "Behaviour of Amyloidogenic Peptides at Liquid Interfaces: Insights from Molecular Dynamics Simulation", 7<sup>th</sup> NUIG-UL conference, NUI Galway, Ireland (Apr 2017).
- [2] "Grand Canonical Transition Matrix Monte Carlo simulations for prediction of Vapour-Liquid Equilibria and Interfacial Properties of TraPPe CO2-Tip4p/2005 Water systems on Atomistically Charged Surfaces", SUNY Buffalo, 17<sup>th</sup> CBE Graduate Research Symposium, NY, USA (Oct 2014).
- [1] "Effect of Oil to Methanol ratio on separation of fatty acids during Transesterification of Rice bran oil", ICACE-2013, NIT Raipur, India (Apr 2013).

## Workshops

- **"Computer Tutorial in Markov Modeling (PyEMMA)"**, Freie Universitaet Berlin, Germany (Feb 2019).
- "CHARMM-GUI CECAM school", EPFL campus, Lausanne, Switzerland (Oct 2018).
- "CCP5 summer school", Lancaster University, UK (Jul 2018).
- "Physics of Life", 49<sup>th</sup> IFF Spring School, FZ Jülich, Germany (Feb 2018).
- "Mapping 3D Objects using a single camera", Stokes Modelling Workshop, NUI Galway, Ireland (Jun 2017).
- "State of the art in mesoscale and multiscale modelling", CECAM-IRL, University College Dublin, Ireland (May 2017).

#### SCHOLASTIC ACHIEVEMENTS

- Awarded Aachen Institute of computational engineering science (AICES) fellowship, RWTH Aachen University, Germany (2018).
- Awarded 120k Class C project CPU hours from Irish High End Computing Centre (ICHEC), NUI Galway, Ireland (2017-18).
- Awarded College of Science (CoS) postgraduate research scholarship, NUI Galway, Ireland (2017).
- Selected for Invitational Internship Program (DAE) at Variable Energy Cyclotron Centre, Kolkata, India (2012).
- Selected for Summer Internship Scholarship Program, NIT Rourkela, India (2011).
- Selected for the 2nd level of Indian National Astronomy Olympiad, India (2005).

## SKILLS

# ■ Scripting Languages

* Python, Bash, Objective C, Swift, Xcode IDE	•••••
* MATLAB, C++, Fortran 2003, Aspen HYSYS, OpenMP, MPI, R	••••

## ■ Visualisation and Molecular modelling tools

* VMD, QTGrace, PyMOL, GROMACS, PLUMED v2.2	•••••
* Gaussian, LAMMPS, CHARMM-GUI	••••

#### ■ Document Preparation and Operating Systems

* LATEX, MS Office, Linux (Ubuntu), MacOS	•••••
* Windows	••••

## ■ Laboratory Equipment and Techniques

* SEM, XRD, FTIR Spectroscopy	, Particle Size Analyzer,	Thermogravimetric analysis	••••