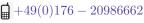
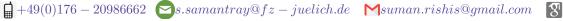


SUMAN SAMANTRAY

IBI-7: Structural Biochemistry, Forschungszentrum Jülich GmbH. Wilhelm-Johnen-Straße, 52425 Jülich, Germany









♥ @samantray_1990





☐ suman - samantray ☐ suman - samantray.github.io ☐



Research Interests

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

EDUCATION

■ AICES fellow, RWTH Aachen University, Aachen, Germany IBI-7: Structural Biochemistry, FZ Jülich GmbH, Jülich, 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 GmbH, 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.
- \triangleright 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

May 8, 2021

- > 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

Sep 2013-Sept 2015

SUNY Buffalo, NY, USA

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

■ Reviewer Jan 2021–present

> Molecular Pharmaceutics, International Journal of Molecular Science

■ Computing Assistant

Aug 2017-Jul 2018

Information Solutions and Services, NUI Galway, Ireland

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, ensuring efficient operationally of all PC suites.

■ 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 display ads fetch SDK users (NBC native apps) and configure it for vendor supply 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

Jul 2017-Aug 2017

Centre for Talented Youth, Dublin City University, Ireland

Dr. Eleanor Healion

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

May 8, 2021 Curriculum Vitae Suman Samantrag

PUBLICATIONS

Peer Reviewed Publications (Total Publications: 6, Total Citations: 23, h-index: 3)



- * equal authorship
- [8] Elucidating the structure of glycosaminoglycans under different physiological conditions, S. Samantray, O.O. Olubivi, B. Strodel, (In preparation), Biomolecules (2021)
- [7] The effects of different glycosaminoglycans on the structure and aggregation of the amyloid-\(\beta\) (16–22) peptide, S. Samantray, B. Strodel, (Under Review), Journal of Physical Chemistry B (2021)
- [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, M. Kaled, B. Strodel, Chemical Science (2021)
- [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) (2021)
- [4] Effect of the air-water interface on the conformation of amyloid beta, S. Samantray, D.L. Cheung, Biointerphases, 15(6), 061011 (2020) (Selected as Featured Article and mentioned in AIP Scilight.)
- [3] Different force fields give rise to different amyloid aggregation pathways in molecular dynamics simulations, S. Samantray, F. Yin, B. Kav, B. Strodel, Journal of Chemical Information and modelling, 60(12), 6462-6475 (2020)
- [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

- [2] "Computational studies on the effects of different cellular environments on amyloid-β aggregation", Hünfeld 2021: Computer Simulation and Theory of Macromolecules, Hünfeld, Germany (Virtual – Apr 2021).
- [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", 5th 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", 3rd Düsseldorf-Jülich Symposium on Neurodegenerative Diseases, Düsseldorf, Germany (Nov 2019).
- [6] "Structure and assembly dynamics of amyloidogenic peptides in aqueous solution and at liquid interfaces", Hünfeld 2019: Computer Simulation and Theory of Macromolecules, Hünfeld, 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", 70th 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", 7th 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, 17th CBE Graduate Research Symposium, NY, USA (Oct 2014).
- [1] "Effect of oil to methanol ratio on separation of fatty acids during trans-esterification of rice bran oil", ICACE-2013, NIT Raipur, India (Apr 2013).

Workshops

- "Computer Tutorial in Markov Modeling (PyEMMA)", Freie Universität 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", 49th IFF Spring School, FZ Jülich GmbH, Germany (Feb 2018).
- "Mapping 3D Objects using a single camera", Stokes Modelling Workshop, NUI Galway, Ireland (Jun
- "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, PyTorch	••••

■ Visualisation and Molecular modelling tools

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

■ Document Preparation and Operating Systems

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

■ Laboratory Equipment and Techniques

* SEM, XRD, FTIR Spectroscopy	, Particle Size Analyzer,	Thermogravimetric analy	sis

REFERENCES

Name:	Prof. (Dr.) Birgit Strodel	Dr. Bogdan Barz	Prof. (Dr.) Gunnar Schroeder
Designation:	Professor	Assistant Professor	Professor
Email:	b.strodel@fz-juelich.de	b.barz@fz-juelich.de	gu.schroeder@fz-juelich.de