



Dr. Suman Samantray, PhD

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RESEARCH INTERESTS

Protein aggregation, Interfacial phenomena, Molecular simulation, Bio-surfactants, Carbohydrate polymers, Phase transition, Machine Learning, Drug discovery, Graph convolutional neural networks

EDUCATION

- **AICES fellow, RWTH Aachen University, Aachen, DEU** Aug 2018 – Nov 2021
Doctor of Philosophy (Dr. rer. nat.) in Computational Engineering Science

Honors : *magna cum laude*

- Dissertation : *Essays on the interplay between glycosaminoglycans and amyloid- β peptides.*
Supervisors : Prof. (Dr.) Birgit Strodel and Prof. (Dr.) Arne Lüchow

- **State University of New York, Buffalo, USA** Aug 2013 – Aug 2015
Master of Engineering (M.Eng.) in Chemical Engineering

- 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, IND** Aug 2009 – Jun 2013
Bachelor of Technology (B.Tech.) in Chemical Engineering

- Dissertation : *Synthesis of activated carbon from agricultural waste for purification of water.*
Supervisor : Prof. (Dr.) Satyabrata Mohanta

RESEARCH EXPERIENCE

- **Ph.D. Researcher** Aug 2018–Aug 2021
IBI-7: Structural Biochemistry, FZ Jülich GmbH, Germany 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** Jan 2017–Jul 2018
School of Chemistry, NUI Galway, Ireland 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

Dept. of Industrial Design, NIT Rourkela, India

Oct 2016–Dec 2016

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

■ Reviewer

Jan 2021–present

- *Molecular Pharmaceutics, MDPI Molecules, MDPI Life*

■ 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, ensuring efficient operationally of all PC suites.

■ Senior Application Developer

*Digital Products and Interactive Media (DPIM) III,
NBC Universal, NY, USA*

Oct 2015–Sept 2016

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

Centre for Talented Youth, Dublin City University, Ireland

Jul 2017–Aug 2017

Dr. Eleanor Healion

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

PUBLICATIONS

Journal articles

* - equal authorship

- [7] **Samantray, S.**, Olubiyi, O.O., & Strodel, B. (2021). The influences of sulphation, salt type, and salt concentration on the structural heterogeneity of glycosaminoglycans. *International journal of molecular sciences*, 22(21), 11529.
- [6] **Samantray, S.**, & Strodel, B. (2021). The effects of different glycosaminoglycans on the structure and aggregation of the amyloid- β (16–22) peptide. *Journal of physical chemistry B*, 125(21), 5511–5525.
- [5] *Paul, A., ***Samantray, S.**, Anteghini, M., Khaled, M., & Strodel, B. (2021). Thermodynamics and kinetics of the amyloid- β peptide revealed by markov state models based on MD data in agreement with experiment. *Chemical science*, 12(19), 6652–6669.
- [4] **Samantray, S.**, & Cheung, D.L. (2021). Effect of the air-water interface on the conformation of amyloid beta. *Biointerphases*, 15(6), 061011. (*Selected as a Featured Article and highlighted in AIP Scilight*)
- [3] **Samantray, S.**, Yin, F., Kav, B., & Strodel, B. (2020). Different force fields give rise to different amyloid aggregation pathways in molecular dynamics simulations. *Journal of chemical information and modelling*, 60(12), 6462–6475.
- [2] Deike, S., Rothmund, S., Voigt, B., **Samantray, S.**, Strodel, B., & Binder, W.H. (2020). β -turn mimetic synthetic peptides as amyloid- β aggregation inhibitors. *Bioorganic chemistry*, 101, 104012.
- [1] Cheung, D.L., & **Samantray, S.** (2018). Molecular dynamics simulation of protein biosurfactants. *Colloids and Interfaces*, 2(3), 39.

BOOK CHAPTERS

- [3] **Samantray, S.**, Schumann, W., Illig, A.-M., Pacheco, M.-C., Paul, A., Barz, B., & Strodel, B. (2022). Molecular dynamics simulations of protein aggregation: protocols for simulation setup and analysis with markov state models and transition networks. In: Li M.S., Kloczkowski A., Cieplak M., & Kouza M. (eds) *Computer Simulations of Aggregation of Proteins and Peptides*, Methods in Molecular Biology, ISBN 9781071615454, vol. 2340, pp. 235–279. Humana Press.
- [2] Olubiyi, O.O., **Samantray, S.**, & Illig, A.-M. (2022). Advances in structure-based virtual screening for drug discovery. In: Tripathi T. & Dubey V. K. (eds) *Advances in Protein Molecular and Structural Biology Methods*, ISBN 9780323902649, pp. 387–404. Academic Press.
- [1] Fatafta, H., **Samantray, S.**, Sayyed-Ahmad, A., Coskuner-Weber, O., & Strodel, B. (2021). Molecular simulations of IDPs: from ensemble generation to IDP interactions leading to disorder-to-order transitions. In: Uversky V. N. (ed) *Progress in molecular biology and translational science*, ISBN 9780323-852999, vol. 183, pp. 135–185. Academic Press.

CONFERENCE PRESENTATIONS

- [2] “**Computational studies on the effects of different cellular environments on amyloid- β aggregation**”. 20th Hünfeld (*Virtual*) Workshop: Computer Simulation and Theory of Macromolecules, Hünfeld, Germany (Apr 2021). →[Videolink](#)
- [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

- [9] “**Simulation studies of amyloid- β peptide and its interactions with glycosaminoglycans**”. EMBO (*Virtual*) Workshop: Advances and Challenges in Biomolecular Simulations (Sep 2021).
- [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**”. 18th Hünfeld Workshop: 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**”. 17th UB 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

- “**3rd Aachen Protein Engineering Symposium (AcES)**”, (*Virtual*) (Sep 2021).
- “**Martini Workshop**”, (*Virtual*) (Sep 2021).
- “**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 2017).
- “**State of the art in mesoscale and multiscale modelling**”, CECAM-IRL, University College Dublin, Ireland (May 2017).

SCHOLASTIC ACHIEVEMENTS

- Graduated Ph.D. with *magna cum laude* from RWTH Aachen University, Germany (2021).
- Awarded bursary to attend and present poster at **EMBO Virtual Workshop: Advances and Challenges in Biomolecular Simulations** (2021).
- 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, Shell/Bash, Tcl, Objective C, Swift, Xcode IDE ●●●●●
- * MATLAB, C++, Fortran 2003, Aspen HYSYS, OpenMP, MPI, R, Julia ●●●●●

■ AI/ ML Tools and Frameworks

- * scikit-Learn, NumPy, pandas, Matplotlib, seaborn
- * PyTorch, TensorFlow, RDKit

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■ Visualisation and Molecular modelling tools

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

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■ Document Preparation and Operating Systems

- * L^AT_EX, MS Office
- * Windows, Linux (Ubuntu), MacOS

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■ Laboratory Equipment and Techniques

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

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OTHER INTERESTS

Cooking, Painting, Reading biographies

REFERENCES

Name:	Prof. Birgit Strodel	Univ.-Prof. Arne Lüchow	Prof. Gunnar Schroeder
Designation:	Professor, HHU Düsseldorf	Professor, RWTH Aachen	Professor, HHU Düsseldorf

Name:	Prof. Jeffrey Errington	Prof. Orkid Coskuner-Weber
Designation:	Professor, SUNY Buffalo	Professor, Turkish-German Univ.

Contact information of scientific referees “available on request”.