
# Dr. Suman Samantray, PhD

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## Research Interests

Amyloid aggregation, Interfacial phenomena, Molecular simulation, 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** *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, MDPI Molecules, MDPI Life*

**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** *Oct 2017–Apr 2018*
*School of Chemistry, NUI Galway, Ireland* Prof. (Dr.) David L. Cheung

- Teaching Assistant for Computational Drug Design and Drug Discovery laboratory, *S*pring 2018
- Teaching Assistant for Physical Chemistry laboratory, *F*all 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.

## 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-$\beta$ 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., Rothemund, 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., IIIig, 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 *Computer Simulations of Aggregation of Proteins and Peptides* (*Methods in Molecular Biology series 2340*, 1st ed., ISBN 9781071615454). Humana Press. (Eds: M.S. Li, M. Cieplak, M. Kouza, & A. Kloczkowski) *In Press*

[2] Olubiyi, O.O., **Samantray, S.**, & Illig, A.-M. (2022). Advances in structure-based virtual screening for drug discovery. In *Advances in Protein Molecular and Structural Biology Methods* (ISBN 9780323902649, pp. 387-404). Academic Press. (Eds: T. Tripathi & V. Dubey)

[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 *Progress in molecular biology and translational science* (ISBN 9780323-852999, Vol. 183, pp. 135-185). Academic Press. (Ed: V. N. Uversky)

## Conference Presentations

[2] **"Computational studies on the effects of different cellular environments on amyloid-β aggregation"**. $20^{th}$ 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"**. $5^{th}$ 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"**. $3^{rd}$ 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"**. $18^{th}$ 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"**. $70^{th}$ 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"**. $7^{th}$ 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 $CO_2$-Tip4p/2005 water systems on atomistically charged surfaces"**. $17^{th}$ 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"**, $49^{th}$ 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, Seaborn ●●●●●
  - PyTorch, Tensorflow, RDKit ●●●○○
- **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 ●●●●●
  - Windows, Linux (Ubuntu), MacOS ●●●●○
- **Laboratory Equipment and Techniques**
  - SEM, XRD, FTIR Spectroscopy, Particle Size Analyzer, Thermogravimetric analysis ●●●○○

## Other Interests

Cooking, Painting, Reading biographies

## References

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|---|---|---|---|
| Name: | Prof. Birgit Strodel | Univ.-Prof. Arne Lüchow | Prof. Orkid Coskuner |
| Designation: | Professor, HHU Düsseldorf | Professor, RWTH Aachen | Professor, Turkish-German Univ. |

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| Name: | Prof. Gunnar Schroeder | Prof. Jeffrey Errington |
| Designation: | Professor, HHU Düsseldorf | Professor, SUNY Buffalo |

**Contact information of scientific referees "available on request".**