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

- **Postdoctoral Researcher / Project Leader** — *Oct 2021–Mar 2022*
  Institute of Biotechnology, RWTH Aachen University, Aachen, DEU — Prof. (Dr.) Ulrich Schwaneberg

  ➢ Development of rational engineering approaches to understand the binding kinetics of anchor peptides (or, adhesion promoting peptides) on polymer surfaces using computational tools and molecular simulations.

  ➢ Co-mentoring of Ph.D. and M.Sc. students in the Computational Biology division.

- **Ph.D. Researcher** — *Aug 2018–Aug 2021*
  IBI-7: Structural Biochemistry, FZ Jülich GmbH, DEU — 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 and Engineering postgraduate fellow *Jan 2017–Jul 2018*
School of Chemistry, NUI Galway, IRL 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, IND 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*
Dept. of Chemical and Biological Engg., 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, IRL 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–May 2016*
Digital Products and Interactive Media (DPIM) III,
NBCUniversal Media, LLC, 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, IRL 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, IRL 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., 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: 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"**. 20^{th} Hünfeld (*Virtual*) Workshop: Computer Simulation and Theory of Macromolecules, Hünfeld, DEU (Apr 2021). →Videolink

[1] **"Behaviour of intrinsically disordered proteins at liquid interfaces: Insights from molecular simulations"**. Nanoscale Simulators Meeting of Ireland, University of Limerick, IRL (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, DEU (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, DEU (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, DEU (Mar 2019).

[5] **"Role of physiological environments in the folding mechanism of intrinsically disordered proteins"**. Biennial Meeting of the German Biophysical Society, Düsseldorf, DEU (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, GBR (Jun 2018).

[3] **"Behaviour of amyloidogenic peptides at liquid Interfaces: Insights from molecular dynamics simulation"**. 7^{th} NUIG-UL conference, NUI Galway, IRL (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, IND (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, DEU (Feb 2019).
- **"CHARMM-GUI CECAM school"**, EPFL campus, Lausanne, CHE (Oct 2018).
- **"CCP5 summer school"**, Lancaster University, GBR (Jul 2018).
- **"Physics of Life"**, 49^{th} IFF Spring School, FZ Jülich GmbH, DEU (Feb 2018).
- **"Mapping 3D Objects using a single camera"**, Stokes Modelling Workshop, NUI Galway, IRL (Jun 2017).
- **"State of the art in mesoscale and multiscale modelling"**, CECAM-IRL, University College Dublin, IRL (May 2017).

Scholastic Achievements

- Graduated Ph.D. with *magna cum laude* from RWTH Aachen University, DEU (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, DEU (2018).

- Awarded 120k Class C project CPU hours from Irish High End Computing Centre (ICHEC), NUI Galway, IRL (2017-18).
- Awarded **College of Science and Engineering postgraduate research scholarship**, NUI Galway, IRL (2017).
- Selected for **Invitational Internship Program (DAE)** at Variable Energy Cyclotron Centre, Kolkata, IND (2012).
- Selected for **Summer Internship Scholarship Program**, NIT Rourkela, IND (2011).
- Selected for the 2nd level of Indian National Astronomy Olympiad, IND (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 ●●●○○
- **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

Name:	Prof. Birgit Strodel	Prof. Gunnar Schroeder	Prof. Jeffrey Errington
Designation:	Professor, HHU Düsseldorf	Professor, HHU Düsseldorf	Professor, SUNY Buffalo
Email:	b.strodel@fz-juelich.de	gu.schroeder@fz-juelich.de	jerring@buffalo.edu

Name:	Prof. Bogdan Barz	Univ.-Prof. Arne Lüchow	Prof. Orkid Coskuner-Weber
Designation:	Professor, HHU Düsseldorf	Professor, RWTH Aachen	Professor, Turkish-German Univ.
Email:	b.barz@fz-juelich.de	luechow@pc.rwth-aachen.de	weber@tau.edu.tr

Please contact Dr. Suman Samantray before requesting references from the scientific referees.