SUMAN SAMANTRAY

IBI-7: Structural Biochemistry,
Forschungszentrum Jülich GmbH,
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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, Germany
  IBI-7: Structural Biochemistry, FZ Jülich GmbH, Jülich, Germany — *Aug 2018 – Aug 2021*
  Doctor of Philosophy (Dr. rer. nat.) in **Computational Biochemistry**

  ➢ Dissertation : Simulation of amyloid aggregation under *in vivo* conditions
  Supervisor : Prof. (Dr.) Birgit Strodel

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

  ➢ 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** — *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, 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 *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

Peer Reviewed Publications (Total Publications: 7, Total Citations: 33, h-index: 4)

* - *equal authorship*

[8] **Samantray, S.** (2021). "Coarse-grained models for intrinsically disordered proteins–carbohydrate polymers interactions". *J. Biomol. Struct. Dyn.*. (*In preparation*)

[7] **Samantray, S.**, Olubiyi, O.O., Strodel, B. (2021). "The influences of sulphation, salt type, and salt concentration on the structural heterogeneity of glycosaminoglycans". *Int. J. Mol. Sci.*. (*Under Review*)

[6] **Samantray, S.**, Strodel, B. (2021). "The effects of different glycosaminoglycans on the structure and aggregation of the amyloid-β (16–22) peptide". *J. Phys. Chem. 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". *Chem. Sci.*, 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", *J. Chem. Inf. Model.*, 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", *Bioorg. Chem.*, 101, 104012.

[1] Cheung, D.L., **Samantray, S.** (2018). "Molecular dynamics simulation of protein biosurfactants", *Colloids Interfaces*, 2(3), 39.

Book Chapters

[3] Olubiyi, O.O., **Samantray, S.**, Illig, A.-M. (2021). "Advances in structure-based virtual screening for drug discovery". *In* T. Tripathi (Ed), Advances in Molecular and Structural Biology of Proteins, Academic Press. (*Under Review*)

[2] 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* V.N. Uversky (Ed), *Prog. Mol. Biol. Transl. Sci.*, Dancing Protein Clouds: Intrinsically Disordered Proteins in the Norm and Pathology, Academic Press, ISBN 9780323852999, Part C, 183, 1st ed. (*In Press*)

[1] **Samantray, S.**, Schumann, W., IIIig, A.-M., Pacheco, M.-C., Paul, A., Barz, B., Strodel, B. (2021). "Molecular dynamics simulations of protein aggregation: protocols for simulation setup and analysis with markov state models and transition networks". *In* M.S. Li, M. Cieplak, M. Kouza and A. Kloczkowski (Eds.), *Methods Mol. Biol.*, Computer Simulations of Aggregation of Proteins and Peptides, Humana Press, ISBN 978-1-0716-1545-4, 2340, 1st ed. (*In Press*)

Conference Presentations

[2] **"Computational studies on the effects of different cellular environments on amyloid-β aggregation"**, Hünfeld 2021(Virtual): 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

[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"**, 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"**, 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"**, SUNY Buffalo, 17^{th} 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"**, 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

- 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 analysis ●●●○○

References

Name:	Prof. (Dr.) Birgit Strodel	Prof. Orkid Coskuner	Prof. (Dr.) Gunnar Schroeder
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Email:	b.strodel@fz-juelich.de	weber@tau.edu.tr	gu.schroeder@fz-juelich.de