SUMAN SAMANTRAY

IBI-7: Structural Biochemistry, FZ Jülich,
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Research Interests

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

Education

- **IBI-7: Structural Biochemistry, FZ Jülich**, Jülich, Germany / ***AICES fellow*, RWTH Aachen University**, Aachen, Germany — *Aug 2018 – present*
  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–Present*
  IBI-7: Structural Biochemistry, FZ Jülich, 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

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 displays ads fetch SDK users (NBC native apps) and configure it for vendors 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 on chemistry experiments to primary and secondary school students.

Publications

[8] **Effect of glycosaminoglycans on the dimerisation pathways of amyloid-βpeptide**, S. Samantray, B. Strodel, (*In preparation*), *Journal of Physical Chemistry B*

[7] **Elucidating the structure of glycosaminoglycans under different physiological conditions**, S. Samantray, O.O. Olubiyi, B. Strodel, (*In preparation*), *Biomolecules*

[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, B. Strodel, (*In Review*), *Chemical Science*

[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)*

[4] **Effect of the Air-Water Interface on the Conformation of Amyloid Beta**, S. Samantray, D.L. Cheung, (*Just accepted*), *Biointerphases*

[3] **Different force fields give rise to different amyloid aggregation pathways in molecular dynamics simulations**, S. Samantray, F. Yin, B. Kav, B. Strodel, (*Just accepted*), *Journal of Chemical Information and modelling*

[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

[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-Juelich Symposium on Neurodegenerative Diseases, Düsseldorf, Germany (Nov 2019).

[6] **"Structure and Assembly Dynamics of Amyloidogenic Peptides in Aqueous Solution and at Liquid Interfaces"**, Computer Simulation and Theory of Macromolecules, Huenfeld, 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 CO2-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 Transesterification of Rice bran oil"**, ICACE-2013, NIT Raipur, India (Apr 2013).

Workshops

- **"Computer Tutorial in Markov Modeling (PyEMMA)"**, Freie Universitaet 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, 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 ●●●●○
- **Visualisation and Molecular modelling tools**
  - VMD, QTGrace, PyMOL, GROMACS, PLUMED v2.2 ●●●●●
  - Gaussian, LAMMPS, CHARMM-GUI ●●●○○
- **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 ●●●○○