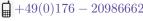


SUMAN SAMANTRAY

IBI-7: Structural Biochemistry, Forschungszentrum Jülich GmbH. Wilhelm-Johnen-Straße, 52425 Jülich, Germany

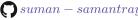




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☐ suman - samantray ☐ suman - samantray.github.io ☐



Research Interests

Amyloid aggregation, Interfacial phenomena, Molecular simulation, Computational Chemistry, 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 Doctor of Philosophy (Dr. rer. nat.) in Computational Biochemistry

Aug 2018 - Aug 2021

- > Dissertation: Simulation of amyloid aggregation under in vivo conditions Supervisor: Prof. (Dr.) Birgit Strodel
- State University of New York, Buffalo, USA Master of Engineering (M.Eng) in Chemical Engineering

Aug 2013 - Aug 2015

> 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 Bachelor of Technology (B. Tech) in Chemical Engineering Aug 2009 -Jun 2013

> 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

IBI-7: Structural Biochemistry, FZ Jülich GmbH, Germany

Aug 2018-Aug 2021 Prof. (Dr.) Birgit Strodel

- > Determination of molecular mechanics parameters and building kinetic transition models to elucidate the amyloid-β aggregation pathways.
- \triangleright 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 School of Chemistry, NUI Galway, Ireland

Jan 2017-Jul 2018 Prof. (Dr.) David L. Cheung

June 29, 2021

- > 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

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, International Journal of Molecular Science

■ 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

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

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.

June 29, 2021 Curriculum Vitae Suman Samantra

PUBLICATIONS

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

- * equal authorship
- [8] Samantray, S., Olubiyi, O.O., Strodel, B. (2021). "A heuristic approach to elucidate the structure of gly-cosaminoglycans with different salt and differing concentrations". Int. J. Mol. Sci. (Under Review)
- [7] 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.
- [6] *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.
- [5] 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. (In Press)
- [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

- [2] Olubiyi, O.O., **Samantray**, **S.**, Illig, A.-M., Strodel, B. (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*)
- 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)

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 glycosamino-glycans", 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).

June 29, 2021 Curriculum Vitae Suman Samantray

- [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", SUNY Buffalo, 17th 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", 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

- 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

Contact information of Professor's who have agreed to write letter of recommendation on my behalf is available on request.