

# Faculty CV

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Profile photo ( 1 photo upto 10 MB)



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Links of Personal webpage/Google scholar/LinkedIn etc.

<https://scholar.google.com/citations?user=plnN8WAAAAAJ&hl=en&oi=ao>

Broad areas of research (only keywords)

Computational Biology; Computational Approach to Produce Smart Materials from Spider Silk Protein;  
Production of BioFuel from Biomass using Microbial Enzymes and Nanomaterials

## Professional Experience

Assistant Professor, Department of Systems and Computational Biology, School of Life Sciences, University of Hyderabad, India, 2020-Present;

UGC-Assistant Professor, Department of Physics, University College of Science, Osmania University, Hyderabad, India, 2014-2020;

DST-SERB Young Scientist, Center for Modeling Simulation and Design (CMSD), University of Hyderabad, India, 2013-2014;

Postdoctoral Research Associate, Department of Chemistry, Michigan State University (MSU), USA, 2011-2013;

Postdoctoral Research Associate, Center for Molecular Biophysics, Oak Ridge National Laboratory, USA, 2007-2010

## Education/Training

Ph.D. (Physical Sciences): Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Thesis title : "Computer Simulation Studies of Supercritical Carbon Dioxide";

M. Sc. (Physics): Science College, Calcutta University, Calcutta, India;

B. Sc. (Physics): St. Xavier's College, Calcutta University, Calcutta, India, 1999

## Detailed research interests (Upto 2 paragraphs or 10 bullet points)

(1) Biofuel Production: Studying microbial enzymes for efficient degradation of cellulosic biomass and its conversion into sustainable biofuels

(2) Smart Materials: Developing spider silk-based hydrogels for biomedical applications, leveraging their behavior in aqueous environments

(3) Biomimetic Materials: Designing self-healing materials like  $\text{CaCO}_3$ , inspired by natural processes

### Selected publications (upto 5)

1. Nanoscale self-assembly and water retention properties of silk fibroin–riboflavin hydrogel

Aarti Kumari, Ganiya Shirin K P, M. Saharay\*

J. Chem. Phys., 162, 024901

(2025) Impact Factor 4.0

it Subject area: Computational Biology

2. Immobilization of Cellulase Enzymes on Single-Walled Carbon Nanotubes for Recycling of Enzymes and Better Yield of Bioethanol Using Computer Simulations

Shubhashree Barik, Akarsh Kumar Dash, M. Saharay\*

Journal of Chemical Information and Modeling, 63, 5192-5203 (2023) Impact factor 6.2

Subject area: Computational Biology

3. Biomolecular interaction of purified recombinant Arabidopsis thaliana's alternative oxidase 1A with TCA cycle metabolites: Biophysical and molecular docking studies

Tadiboina Veera Sankar, M. Saharay, Dharawath Santhosh, Saji Menon, Sreejith Raran-Kurussi, Kollipara Padmasree

International Journal of Biological Macromolecules, 258, 128814 (2023) Impact factor 8.025

Subject area: Experimental Biology

4. CelS-catalyzed Processive Cellulose Degradation and Cellobiose Extraction for Production of Bioethanol

Sree Kavya Penneru, M. Saharay\* , Marimuthu Krishnan

Journal of Chemical Information and Modeling,

DOI: (<https://doi.org/10.1021/acs.jcim.2c00239>) (2022) Impact factor 6.2

Subject area: Computational Biology

5. Formation of Amorphous Precursor Phase in the Biomineralization of Calcium Carbonate Mediated by Avian Egg-shell Protein

R. Sandya Rani, M. Saharay

RSC Advances, 9, 1653-1663 (2019) Impact factor 3.12

Subject area: Computational biology

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### Selected projects (upto 5)

Principal investigator (PI) for the project entitled "Computational Approach to Produce Smart Materials from Spider Silk Protein"

Amount : Rs. 26,00,000

Sponsor : CSIR, India

Duration : 2025-2028

Principal investigator (PI) for the project entitled "Production of BioFuel from Biomass using Microbial Enzymes and Nanomaterials: A Computational Study"

Amount : Rs. 22,00,000

Sponsor : Institute of Eminence (IoE), Govt. of India

Duration : 2022-2024

### Selected patents (a paragraph or upto 5 bullet points)

None

### Current PhD scholars and broad research topics

1. Shubhashree Barik is working on 'Production of BioFuel from Biomass using Microbial Enzymes and Nanomaterials'

2. Aarti Kumari is working on 'Computational Approach to Produce Smart Materials from Spider Silk Protein'

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