

SHIKHA MALICK

AI Researcher

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📍 New Delhi, India

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🔗 mshik

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TECHNICAL SKILLS

Python

C++

C

ROS

CUDA

PyTorch

MXNet

TensorFlow

OpenCV

NumPy

Pandas

Matplotlib

SKLearn

TensorRT

GNN

Drug Discovery

Healthcare

Computer Vision

Multimodal AI

Generative AI

Git Versioning

Docker

ACHIEVEMENTS

Winner "AI in Healthcare Hackathon"

📅 August 2021 📍 SINE IITB

University Scholarship for Summer Internship

📅 June 2016 📍 AIT Bangkok

REFERENCES

[Dr. Sahely Bhadra](#)

Associate Professor, IIT Palakkad

✉ sahely@iitpkd.ac.in

[Dr. Mrinal Das](#)

Assistant Professor, IIT Palakkad

✉ mrinal@iitpkd.ac.in

[Dr. Deepak Rajendraprasad](#)

Associate Professor, IIT Palakkad

✉ deepak@iitpkd.ac.in

PUBLICATIONS

• **CDGCN: Conditional de novo Drug Generative Model Using Graph Convolution Networks** 🌐

Shikha Mallick and Sahely Bhadra

📅 3 April 2023

📍 RECOMB 2023, Istanbul, Turkey

• **Solubility prediction of industrial chemicals: Feeding Graph Neural Networks with physics-based simulations data** 🌐

Shikha Mallick et al.

📅 28 April 2023

📍 AIChE Spring meeting 2023, Houston, US

EXPERIENCE

Machine Learning Engineer | [Siemens Digital Industries Software](#)

📅 March 2022 – Present

📍 Pune, India

- 3D Shape Recognition using Multimodal AI
- Molecular Solubility Prediction using GNN and Multimodal AI
- Onsite project in Japan on Perception & Sensor Fusion using Late fusion methods
- Real-life Scene Generation using Generative AI
- 3D fault detection using Explainable AI

EDUCATION

MS by Research (CS) | [Indian Institute of Technology, Palakkad](#)

📅 July 2019 – July 2022

📍 Palakkad, India

- CGPA: 8.4
- Thesis: **Graph Generative Network for Novel Protein-specific de novo Drug Generation**
- Teaching Assistant: **Deep Learning Lab** | **Machine Learning Lab** | **Data Engineering Lab** | **Programming Lab**

Bachelor of Tech. (CS) | [Dr. A.P.J. Abdul Kalam Technical University](#)

📅 August 2013 – June 2017

📍 Lucknow, India

- Percentage: 78.4
- Project: **Timetable Generation using Genetic Algorithm in Java**

PROJECTS

CDGCN | 🌐

📅 March 2022

- Official implementation of the [CDGCN](#) paper

XGB-EVM | 🌐

📅 August 2021

- First prize in "AI for Healthcare Hackathon", SINE IITB & DERBI Foundation
- Deep ensemble model for the detection of eye diseases from FUNDUS retina images