


# AGNEY K RAJEEV

Integrated MSc. Fourth  
Year

 Bhubaneswar, India

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 AKR211

## EDUCATION

### National Institute of Science Education and Research

INT MSc 2026

- Major in **Physics**
- Minor in **Computer Science**
  - Current CGPA: **9.03**

Bhubaneswar, India

10/2021 - present

### Chinmaya Vidyalaya Kolazhy

HIGHER SECONDARY SCHOOL 2021

- Class XII CBSE 2021: 97.0 percent
- Class X CBSE 2019: 95.0 percent

Thrissur, India

2009-2021

## INTERNSHIPS/PROJECTS

### Computational Studies of The Ising Model

SUMMER INTERNSHIP

- Monte Carlo Simulation
- Ising Model
- Numpy
- Matplotlib

NISER, Bhubaneswar

2/6/2023 - 31/7/2023

The Internship was carried out under the guidance of Dr. A. V. Anil Kumar of NISER. We conducted a study of the 2D Ising model implemented using the Metropolis Algorithm to observe parameters such as Energy, Net Magnetization, Specific Heat Capacity, Magnetic Susceptibility etc. and determined the existence of a phase transition in the model. Using results from above we attempted to incorporate non reciprocal interactions and random fields to the model and observe any change in results.

[Source Code](#)

[Project Report](#)

[Certification](#)

### Physics Informed Neural Networks with PyTorch

SEMESTER PROJECT

- Machine learning
- Physics Informed Neural Networks
- PyTorch

NISER, Bhubaneswar

1/7/2023 - 27/11/2023

The project was carried out as part of the Computational Physics Lab Course. We aimed to develop a Physics Informed Neural Network (PINN) to solve Differential Equations (DEs) using Machine Learning.

[Source Code](#)

[Project Report](#)

[Presentation](#)

### Predicting Protein Oligomericity from Amino Acid Sequence

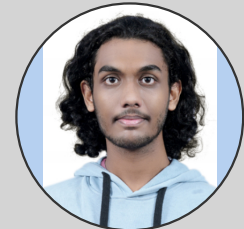
SEMESTER PROJECT

- Machine Learning
- Dataset Curation
- kNN, Random Forest, Transformers
- sklearn, PyTorch, Pandas

NISER, Bhubaneswar

2/1/2024 - 7/9/2024

This project was carried out under the supervision of Dr. Subhankar Mishra in connection with the Machine Learning course. We aimed to create a machine learning model for predicting the oligomerization states possible for the amino



## ABOUT ME

NISERite, Aspiring Computational Physicist, Hobbyist Coder, Amateur Keyboardist

**Research Interests:** Molecular simulations, Machine Learning, Biological systems, Active matter, Non-reciprocal interactions

## PROGRAMMING

Base Python

Numpy

Scipy

PyTorch

Pandas

Julia

MATLAB

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## LANGUAGES

**Malayalam** • Mother tongue

**English** • Fluent

**Hindi** • Fluent

## HOBBIES

- Table Tennis, Chess
- Playing Keyboard
- Coding, Cryptographic puzzle solving

acid sequence of a protein. We achieved near state-of-the-art results in classifying fluorescent proteins into monomers and oligomers. The results are currently under review for the NLDL conference 2025.

[Proposal Presentation](#)

[OpenReview](#)

### **Predicting the Stress Tensor for a simulated molecular system** *IISER, Kolkata*

SUMMER INTERNSHIP

14/5/2024 - 14/7/2024

- Machine Learning
- Graph Neural Networks
- Dataset Generation
- Pytorch, PyG

The project was conducted under the supervision of Dr. Neelanjana Sengupta in her lab at IISER Kolkata. Our goal was to predict the Cauchy stress tensor of a molecular system using deep learning techniques as a more efficient alternative to the traditional computation method based on pairwise atomic interactions, which is inherently time-consuming. We successfully obtained novel preliminary results for the atomic stress tensor of a water box by applying node regression learning in graph neural networks.

[Project Report](#)

[Certification](#)

## **HIGHLIGHTS**

### • **Published Preprint**

Published preprint on [Ising model with non-reciprocal interactions](#) with Dr. A. V. Anil Kumar based on the results obtained during my first summer internship

### • **Submitted paper to conference**

Submitted paper titled [Predicting Oligomeric states of Fluorescent Proteins using Mamba](#) with Joel Joseph K B and Dr. Subhankar Mishra to Northern Lights Deep Learning Conference 2025 (currently under review)

## **HONOURS**

2023	<b>Topper</b> , Semester IV, School of Physical Sciences	<i>NISER, Bhubaneswar</i>
2021	<b>Scholar</b> , Innovation in Science Pursuit for Inspired Research (INSPIRE)	
2021	<b>Top 6</b> , Indian Olympiad Qualifier in Mathematics (Kerala Region)	
2021	<b>99.16 percentile</b> , JEE Main	
2021	<b>Rank 186</b> , IISER Aptitude Test (IAT)	
2021	<b>Rank 174</b> , National Entrance Screening Test (NEST)	
2021	<b>Among 1 percent of successful candidates</b> , CBSE XII	<i>Delhi, India</i>
2019	<b>Cleared the Aptitude Test</b> , KVPY SA	

## **COURSES**

The relevant courses I undertook are given below

**Physics** : Classical Mechanics I, Mathematical Methods I & II, Quantum Mechanics I & II, Statistical Mechanics, Introduction to Condensed Matter Physics, Classical Mechanics II (ongoing), Non-equilibrium Statistical Mechanics (ongoing)

**Computer Science** : Introductory Python Programming I & II, Theory of Computation, Discrete Structures and Computation, Design and Analysis of Algorithms, Machine Learning, Complexity Theory (ongoing)

I have also completed Introductory courses in Chemistry, Biology, Maths and Humanities