


# SUBHAJIT ROY

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 1050 S Stanley Pl #P213, Tempe, AZ, 85281

## EDUCATION

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### Physics, PhD

Petr Sulc's Lab, Arizona State University

Computational design and analysis of genetic materials, focusing on self-assembly.

*August 2022 - Present*

Current CGPA - 4/4

### Physics, Integrated BS-MS

UM-DAE-Centre For Excellence In Basic Sciences

PLAS-5k binding affinity database and retrosynthesis prediction using Deep Learning, Prof Deva Priyakumar, IIIT Hyderabad

Entropic theoretical study of  $\beta$  ladder domain of Zika Virus

*August 2017 - July 2022*

Current CGPA - 7.3/10

### Senior Secondary Education

D.A.V. Public School, Rupnarayanpur

*April 2015 - May 2017*

Score - 84.6%

### Secondary Education

Burnpur Riverside School, Chittranjan

*March 2015*

CGPA - 10/10

## RESEARCH EXPERIENCE

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### • Coarse Grain DNA Origami Model

*2022-Present*

Designing a coarse grain representation of DNA origami using heterogeneous anharmonic oscillator and Patchy Particle model reducing computational time by 100 times still maintaining underlying statistical features using oxDNA with vanilla C

### • Seeding DNA Origami Growth

*2022-Present*

Achieved higher yield and self growth of DNA origami crystals using pre-assembled origami particles experimentally, guided by simulation prediction.

### • DNA-PAINT data analysis via oxDNA prediction

Collaborated with experimental group to help them analyse their experimental data generated using DNA-PAINT and de-convolute complicated 3D geometry of the origami used in the experiment. This analysis even improved the resolution to approximately 1nm and shed light on its dynamics.

### • PLAS-5k Database

Created 5000 protein ligand complex database using MD simulation in aqueous environment and reported various important properties like polar, non-polar interaction, electrostatic interaction, Van Der Waals' interaction. Results outperformed commonly used docking tool Auto Dock Vina, and strongly believe that this would be highly helpful to ML studies related to protein-ligand complexes and docking.

### • Potential destabilizing hotspot in the $\beta$ ladder domain of ZIKA

Established bio-chemical pathway to destabilise one of the essential proteins of ZIKA virus by cleaving di-sulphide bond in the  $\beta$  ladder domain of NS1 protein, which is responsible for its growth and infection via surface attachment and many other essential functions. This was concluded using extensive thermodynamics study.

### • Observational Radio Astronomy

### • Projects performed under guidance of Prof. R Nagrajan

*2018-2019*

– Modeled Clustered computer in heterogeneous environment using Raspberry Pis.

8 Raspberry Pis connected in a random configuration using both LAN and wireless were used simultaneously to perform a parallel task with unequal distribution. The distribution of the task dependant on various factors including latency, previous performance etc. A complex algorithm was put to use to make use of both the GPU and CPU using OpenCL and C++.

TECHNICAL SKILLS

<b>Programming:</b>	Python, C++ (including CUDA and MPI), FORTRAN, MATHLAB, Bash, Java, R, JS, C#, Lua
<b>Software &amp; Tools:</b>	<b>Simulation Platform:</b> NAMD, GROMACS,Amber20,OpenMM,OxDNA
	<b>Visualizing Software :</b> VMD, UCSF Chimera, Pymol, OxDNA-viewer(Oxview)
	<b>Non-Accademic Platforms:</b> Gatsby(React) JS, Laravel, Lumen, NodesJs Backend, Unity
	Android(Java), React Native, Flutter(Android and IOS)
	<b>Others:</b> Tensorflow, Keras, PyTorch, Embedded C (Arduino and STM32), Raspberry PI

PUBLICATION/PRE-PRINT

1. Roy P, Roy S, Sengupta N. Disulfide Reduction Allosterically Destabilizes the  $\beta$ -Ladder Subdomain Assembly within the NS1 Dimer of ZIKV. Biophys J. 2020 Oct 20;119(8):1525-1537.

2. Korlepara, D.B., Vasavi, C.S., Jeurkar, S. , Pal, Pradeep, Roy, Subhajit et al. PLAS-5k: Dataset of Protein-Ligand Affinities from Molecular Dynamics for Machine Learning Applications. Sci Data 9, 548 (2022).

3. High-speed 3D DNA-PAINT and unsupervised clustering for unlocking 3D DNA origami cryptography G. Bimananda M. Wisna, Daria Sukhareva, Jonathan Zhao, Deeksha Satyabola, Michael Matthies, Subhajit Roy, Petr Šulc, Hao Yan, Rizal F. Hariadia bioRxiv 2023.08.29.555281

AWARDS AND ACHIEVEMENTS

- Recipient of DST-INSPIRE fellowship under SHE schemes (2017-2022)
- Vijyoshi Science Camp-2018 organized by KVPY, at IISC, bangalore.
- Science Olympiad Silver zone- 2014 (Gold Medalist).
- School topper in 10th.

CONFERENCES AND WORKSHOP ATTENDED

- Journal of Physical Chemistry Workshop, at IISER Kolkata, June, 2018.
- AWS World Summit Online 2020, 13th May.
- Science Leadership Workshop – 2020.
- Big Data 2020, Centre For Mathematical Sciences and Applications, Harvard University.