

## Junior Research Fellow (JRF) position under DST-SERB funded project

Applications are invited for the position of Junior Research Fellow in the Department of Chemical Engineering at BITS Pilani, K. K. Birla Goa Campus, Goa for DST-SERB sponsored research project titled "Determination of the protein folding, unfolding and refolding of spike glycoprotein of SARS Corona Virus-2 in Rubik's Cube based statistical model and study of the thermodynamic interaction and kinetic behavior of the various equilibrated conformations with receptor of angiotensin converting enzyme-2 (ACE-2)" DST-SERB-POWER (FILENO. SPG/2021/004541).

## **Objectives of the Project:**

(i) Develop a Rubik's Cube Model (RCM) based simulation technique to understand the folding, unfolding and refolding kinetics and various protein folding pathways of Severe Acute Respiratory Syndrome Coronavirus-2 (SARS-COV2) spike glycoprotein. (ii) Study of protein-folding dynamics of spike glycoprotein with statistical energy landscape theory (SELT) based stochastic model. (iii) Compare the similarity and dissimilarity between SELT and RCM model in details to understand the formation of various types of spike glycoprotein conformations and the efficiency of the Rubik's Cube model. (iv) Calculation of the mean first-passage time (MFPT) using both SELT and RCM model at different temperature. (v) Understand the thermodynamics of molecular interaction between spike glycoprotein and the newly obtained equilibrated folded-unfolded-refolded conformations with receptor of angiotensin-converting enzyme-2 (ACE-2) using Grand Canonical Monte Carlo (GCMC) Simulation and calculation of the binding energy.

## Principal Investigator: Dr. Paramita Haldar Broad area of Research: Molecular Modeling in Chemical Engineering Duration of the project: 3 Years

Fellowship Amount (Rs.): Rs. 31,000 (1<sup>st</sup> Year and 2<sup>nd</sup> Year) and Rs. 35,000 (3<sup>rd</sup> Year)

**Accommodation:** Hostel accommodation will be provided subject to availability and will be governed by the rules and regulations of the Institute prevailing at the time of joining of the candidate.

**Qualification (Compulsory):** Post Graduate Degree in Basic Science OR Post Graduate in Degree in Engineering selected through a process described through any one of the following:-

- 1. Scholars who are selected through National Eligibility Tests- CSIR –UGC NET including lectureship (Assistant Professorship) and GATE. Without Net/GATE score applications will not be considered.
- 2. The Selection process through National level examinations conducted by central Government departments and their agencies and Institutions such as DST, DBT, DAE, DOS, DRDO, MHRD, ICAR, IIT, IISc, IISER etc.

## **Qualification (Desired):** Knowledge of programming (Matlab/Fortran/Python)

How to Apply: Interested candidates may send current curriculum vitae with details of research experience to the principal investigator (email: <u>paramitah@goa.bits-pilani.ac.in</u> OR <u>paramita.haldar82@gmail.com</u>) by 31<sup>st</sup> July, 2022. Only shortlisted candidates will be contacted via e-mail for online/Personal interview to be held at BITS Pilani, Goa Campus and no TA/DA will be paid for the Interview.

Selected candidate may get a chance to apply for PhD degree at BITS Pilani, K. K. Birla Goa Campus (Rules of PhD program for BITS Pilani are applicable)

