

Anji Babu Kapakayala

Department of Chemistry

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Date of Birth: 08th May 1991

Nationality: Indian

Ph.D. Status: Expected to submit thesis in 1 month



Education

PhD in Computational Biophysical Chemistry

2015–present

A joint Ph.D. program,

Department of Chemistry,

Indian Institute of Technology Kanpur, India

Thesis Advisor: Prof. Nisanth N. Nair

School of Pharmacy and Biomedical Sciences,

Curtin University, Perth, Australia.

Co-supervisor: Prof. Ricardo L. Mancera

Thesis Title: **Boosting the Conformational Sampling of Biomolecular Systems: Novel Hybrid Local and Global Enhanced Sampling Approaches**

CGPA:8.33/10

Research Assistant

2014–2015

Department of Inorganic and Physical Chemistry,

Indian Institute of Science Bangalore, India.

Project Title: Computational study of structural and electronic properties of 2D layered materials and their electrochemical applications like Hydrogen Evaluation Reaction (HER) and Oxygen Reduction Reaction (ORR).

Under Supervision of Prof. S. Sampath

M.Sc. in Chemical Sciences

2011–2013

Department of Chemistry,

Pondicherry University, India.

M.Sc. Project Title: Distortions in oxidised hydro phorphyrine analogs and its aromatic pathway.

Under Supervision of Dr. M. M. Balakrishna Rajan

CGPA: 7.64/10

B.Sc. in Chemistry, Physics and Mathematics

2008–2011

Andhra University, Andra Pradesh, India.

Percentage: 70.0%

Research Interests

- Development of enhanced sampling methods in combination with machine learning approaches.
- Development of methods to find reaction coordinates using machine learning techniques.
- Development of software and tools related to Molecular Dynamics.
- Molecular level understanding of intricate biological processes having potential application in medicinal science and molecular biology. That include
 - Protein-drug binding/unbinding process
 - Protein - Protein interactions
 - Intrinsically disordered proteins (IDPs)
 - Membrane small molecule binding/unbinding process

Expertise

- Modelling bio-molecular simulations.
- Molecular dynamics (MD) simulations.
- Deep understanding of enhanced sampling techniques – (a) Umbrella Sampling (b) Metadynamics (c) Temperature accelerated Molecular Dynamics (d) Well-Sliced Metadynamics and TASS (a combined approach of umbrella sampling, metadynamics and TAMd) (e) Replica exchange molecular dynamics (REMD) and its variants like REST2.
- Packages: AMBER, GROMACS, PLUMED, Gaussian 09, Mathematica 07, SHIFTX2, VASP, Material Studio, and visualization packages (VMD and Molden)
- Programming Skills: Fortran, MPI programming, Bash/Shell Scripting, TCL-VMD Scripting, C++ and Python.
- Developer Tools: git, Github, Docker-containers,
- Linux server administration skills.
- Website designing skills: Google sites and Bootstrap studio 5.1.

Packages written

- **REWEIGHT:** Is a module based fortran package to perform reweighting for various enhanced sampling methods like TASS, WSMTD, MTD, US etc.
Github repository:
https://github.com/anjibabuIITK/TASS_REWEIGHTING_PACKAGE
- **Clustering:** is a program to perform cluster analysis using VMD written in TCL language. Performs the clustering based on the RMSD using VMD measure cluster keyword within given RMSD cutoff.
Github Repository:
<https://anjibabuiitk.github.io/CLUSTER-ANALYSIS-USING-VMD-TCL>

- **Easy Console Tool:** Performs many trajectory analysis through VMD console written in TCL.
Github repository: <https://github.com/anjibabuIITK/EasyConsoleTool/releases/tag/v1.0.0>
- **Keys:** is a personal password manager written in Shell language to help a user to store and organize passwords. Keys manages and stores the passwords encrypted and locally, requiring the user to create a master password.
Github repository: https://github.com/anjibabuIITK/Keys-The_Password_Manager/releases/tag/1.0
- **Rbin:** is a simple and user-friendly package written in shell to act as a command-line recycle-bin for Linux. Github repository: https://github.com/anjibabuIITK/RECYCLEBIN_for_Linux/releases/tag/v1.0

Tutorials Written

- **REMD:** A tutorial on setting up the replica exchange molecular dynamics (REMD) simulation using alanine dipeptide as a toy model.
Github repository: [Click Here](#)
- **REST2:** A tutorial on replica exchange solute scaling (REST2) using alanine dipeptide in explicit water as a toy model. Github repository: [Click Here](#)
- **Enhanced Sampling Methods:** A repository for tutorials of enhanced sampling methods. Github repository: https://github.com/anjibabuIITK/Enhanced_Sampling_Methods_Tutorials

Experience on Machine Learning

- **Steepest Descent Algorithm:** Minimization algorithm for simple harmonic potential.
Github repository: https://github.com/anjibabuIITK/Python_Programs/tree/master/Steepest_Descent_Minimisation
- **Gaussian Regression:** A program to approximate the given free energy profile with Gaussian functions.
- **Kernal Density Compression Algorithm:** Wrote a model program for KDC algorithm.
Github repository: https://github.com/anjibabuIITK/Kernel_Density_Compression_Algorithm
- **Speeding-up the Bias Calculation in Metadynamics using Nearest Neighbours:** [To be published](#)

List of Publications

1. "Boosting the Conformational Sampling by Combining Replica Exchange with Solute Tempering and Well-Sliced Metadynamics.", **Anji Babu Kapakayala** and Nisanth N. Nair, *J. Comput. Chem.*, **2021**.
2. "Free energy calculations of alanine tripeptide in explicit water using temperature accelerated sliced sampling.", **Anji Babu Kapakayala**, Abhinav Gupta, Shivani Verma and Nisanth N. Nair, *J. Indian Chem. Soc.*, 96, 875-882, **2019**.

3. "Enhancing the Hidden Slow Motions in the Temperature Accelerated Sliced Sampling by Combining with Replica Exchange Solute Scaling.", **Anji Babu Kapakayala** and Nisanth N. Nair, *Manuscript under preparation*.
4. "Investigating the Crucial Interactions in Unbinding of Meropenem from New Delhi Metallo β Lactamase.", **Anji Babu Kapakayala** and Nisanth N. Nair, *Manuscript under preparation*.
5. "Structural Characterization of Intrinsically Disordered Proteins by Parallely Biased Replica Exchange Solute Tempering.", **Anji Babu Kapakayala**, Nisanth N. Nair, and Ricardo L. Mancera, *Manuscript under preparation*.

Conferences

- Recent Advances in Modeling Rare Events (RARE-2021), online, India, Dec, 2021.
- Theoretical Chemistry Symposium (TCS), IISER Kolkata, online, India, December, 2021.
- Research Scholars Day (RSD-2021), Department of Chemistry, IIT Kanpur, India, Aug 2021.
- Association of Molecular Modellers of Australia (AMMA-2019), Indonesia, Dec, 2019.
- Western Australia Computational Chemistry Conference (WACCC-2019), Perth, Australia, Nov, 2019.
- Recent Advances in Modeling Rare Events (RARE-2017), Agra, India, Dec, 2017.
- Participated in National Conference in Frontier Areas of Chemistry 2011 (NCFAC 2011).
- Participated in Chemical Research Society of India South Zonal Meeting on Dec 16-17, 2011.

Teaching Experience

- CHM-102A ("General Chemistry" for B. Tech. program, Jan 2020), Department of Chemistry, IIT Kanpur.
- CHM-421A ("Quantum Chemistry" for M.Sc. program, June 2018), Department of Chemistry, IIT Kanpur.

Awards

- Received "CIPRS and Research Stipend Scholarship" grant to work at Curtin University, Australia in 2019.
- Qualified GATE (Graduate Aptitude Test in Engineering) in Chemistry in 2014 and 2015.
- Qualified CSIR-NET for Ph.D. entrance conducted by CSIR (Council of Scientific & Industrial Research) India in December 2013.
- Secured 19th rank in M.Sc. Entrance exam conducted by Andhra University in 2011.
- Secured 96th rank in M.Sc. Chemical sciences entrance exam conducted by Pondicherry University in 2011.

Reference

- Prof. Nisanth N. Nair
Thesis advisor
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Indian Institute of Technology Kanpur
Kanpur – 208016, UP, India
Tel: 0512-259-6311
Email: nnair@iitk.ac.in
- Prof. Ricardo L. Mancera
Co-Supervisor
School of Pharmacy and Biomedical Sciences,
Curtin University,
Perth, Australia
Tel: 08 9266 1017
Email: R.Mancera@curtin.edu.au

Declaration

I hereby declare that the information compiled above is precise & accurate in its entirety and the requisite documents/certificates can be produced at any time.



Anji Babu Kapakayala