Praveen Kumar, Ph.D. (he/him/his)

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Personal Information

Nationality: Indian
Date of Birth: 10 May 1994
Gender: Male
Marital Status: Single

Current Affiliation

I am working with Prof. Rajarshi Chakrabarti as a Postdoctoral Fellow in the Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400076, India.

PhD Advisor

Prof. Rajarshi Chakrabarti
Department of Chemistry
Indian Institute of Technology Bombay
Mumbai 400076, India
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Doctoral Degree Details

- Area: Tracer dynamics in crowded and complex environments
- Thesis Title: "*Understanding the Dynamics of Active and Passive Probe Particles in Complex Environments using Computer Simulations*"
- Thesis submitted: November 2022
- Awarded: February 2023

Education

Degree	Year	Institution/University	Division
Ph.D. (Physical Chemistry)	2023	Indian Institute of Technology Bombay	
M.Sc. (Chemistry)	2017	National Institute of Technology, Jalandhar	First
B.Sc.(Mathematics) Physics, Chemistry	2015	Central University HNBGU, Uttarakhand	First

Research Experience

- I conducted research for my M.Sc. final-year project on "*Photocatalytic degradation of methylene blue by poly(methyl methacrylate)/metal oxide nanocomposites*" under the supervision of Prof. Uma Shanker at the Department of Chemistry, National Institute of Technology Jalandhar, Punjab, India.
- Additionally, I completed a summer internship during my M.Sc. under Prof. P. P. Thankachan at the Department of Chemistry, Indian Institute of Technology, Roorkee, Uttarakhand, India, where I explored "*Computational Studies on Electric Properties of Trans-Stilbene Derivatives using Gaussian 09 software.*"

Publications

1. **Praveen Kumar**, Ligesh Theeyancheri, Subhasish Chaki and Rajarshi Chakrabarti, *Transport of probe particles in polymer network: effects of probe size, network rigidity, and probe-polymer interaction*, Soft Matter **15**, 8992 (2019). **Featured on the back cover**.

2. **Praveen Kumar**, Ligesh Theeyancheri and Rajarshi Chakrabarti, *Chemically symmetric and asymmetric self-driven rigid dumbbells in a 2D polymer gel*, Soft Matter **18**, 2663 (2022).

3. Ligesh Theeyancheri, Rajiblochan Sahoo, **Praveen Kumar**, and Rajarshi Chakrabarti, *In silico studies of active probe dynamics in crowded media*, ACS Omega **7**, 33637 (2022)**(Invited Mini-Review).**

4. **Praveen Kumar** and Rajarshi Chakrabarti, *Dynamics of self-propelled tracer particles inside a polymer network*, Phys. Chem. Chem. Phys. **25**, 1937 (2023).

5. **Praveen Kumar** and Rajarshi Chakrabarti, *Escape dynamics of a self-propelled nanorod from circular confinements with narrow openings*, Soft Matter **19**, 6743 (2023).

6. **Praveen Kumar**, Ramanand Singh Yadav and Rajarshi Chakrabarti, *Brownian dynamics simulations of the self-propelled rod-shaped tracers in complex media: rotational and translational diffusion* (Manuscript under preparation).

7. Ramanand Singh Yadav, **Praveen Kumar**, Valerio Sorichetti, Mehdi Bouzid, and Rajarshi Chakrabarti, *Structure and dynamics of densely-packed active Brownian particles in presence of obstacles* (In preparation).

COMPUTATIONAL TECHNIQUES

Langevin/Brownian Simulations - apply for coarse-grained modeling of various functional soft materials and study of active and passive probes through these complex and crowded environments.

SUMMARY OF RESEARCH WORK

The dynamics of tracer particles in crowded and complex environments, such as biological hydrogels, polymer matrices (networks, solutions, or melts), and confinements with narrow openings, is a subject of fundamental interest in many scientific fields, including biophysics, materials science, chemistry, and medical engineering. These tracers could be passive, such as colloids, or active (self-propelled), such as synthetic nanomotors or bacteria. Apart from the motion at the single particle level in crowded media, the collective motion of active particles or active polymers is also of prime importance. We use coarse-grained Langevin/Brownian dynamics simulations as the tools for our study.

- **Transport of passive probe particles in 3D polymer network**
  Based on extensive molecular dynamics simulations, we have investigated the dynamics of tracer beads in a polymer network created on a diamond lattice, which provides substantial crowding like the cellular environment. From the time-and-ensemble averaged translational mean square displacement, van Hove correlation functions, and angular distribution functions, we have shown that the dynamics of the probe increasingly becomes restricted, non-Gaussian, and subdiffusive on increasing the network rigidity, binding affinity, and probe size. In addition, in a short time, the velocity autocorrelation functions have negative dips owing to caging of the probe, where fractional Brownian motion (FBM) and continuous time random walk (CTRW) both contribute. Importantly, for a probe particle of size comparable to the mesh size, unrestricted motion engulfing large-length scales has been observed. This happens with a more flexible polymer network, which is easily pushed by the bigger probe. On increasing the rigidity of the network, the bigger probe can not efficiently push the network, and as a result, the long tail disappears. This study gives a general qualitative picture of the passive transport of probes in a gel-like medium, as encountered in different contexts.

- **Chemically symmetric and asymmetric self-driven rigid dumbbells in a 2D polymer gel**
  We employ overdamped Langevin simulations to unveil the translational and rotational dynamics of self-driven chemically symmetric and asymmetric rigid dumbbells in a two-dimensional polymer gel. Our results show that the activity or the self-propulsion always enhances the dynamics of the dumbbells. Making the self-propelled dumbbell chemically asymmetric leads to further enhancement in dynamics. Additionally, the direction of self-propulsion is a key factor for chemically asymmetric dumbbells, where self-propulsion towards the non-sticky half of the dumbbell results in faster translational and rotational dynamics compared to the case with the self-propulsion towards the sticky half

of the dumbbell. Our analyses show that both the symmetric and asymmetric passive rigid dumbbells get trapped inside the mesh of the polymer gel, but the chemical asymmetry always facilitates the mesh-to-mesh motion of the dumbbell, and it is even more pronounced when the dumbbell is self-propelled. This results in multiple peaks in the van Hove function with increasing self-propulsion.

- **Dynamics of self-propelled tracer particles inside a polymer network**
  Motivated by the transport phenomena of biomolecules, bacteria, and synthetic nanomotors through mesh-like environments such as mucus membranes, nuclear pore complexes, and porous media, we construct a polymer network on a diamond lattice and use computer simulations to investigate the dynamics of spherical self-propelled particles inside the network. Our main objective is to elucidate the effect of the self-propulsion on the dynamics of the tracer particle as a function of the tracer size and stiffness of the polymer network. We compute the time-averaged mean-squared displacement and the van-Hove correlations of the tracer. Our results show that the dynamics of the self-propelled tracer crossover short-time subdiffusion to an intermediate-time superdiffusion. This happens due to a tug-of-war between the suppressed motion of the tracer inside a mesh and its tendency to escape from it due to self-propulsion. Interestingly, the bigger tracers, if sticky, show stronger subdiffusion and, if active, also exhibit stronger superdiffusion compared to a tracer of smaller size. In addition, the stiffness of the network largely affects the dynamics of the tracer with the bigger and comparable size to the polymer mesh; the stiffer the network, the slower the dynamics of the tracer.

- **Escape dynamics of a self-propelled nanorod from circular confinements with narrow openings**
  In the context of diffusive transport inside the cellular environment, a particle is often confined to a domain with small openings present on the boundary. Examples include ions transport through ion channels in and out of cells, intercellular transport of proteins between the cytoplasm and the nucleus through nuclear pore complex (NPC), proteins moving between the meshes of the mucus membrane, and bacteria motion through disordered media where it moves between the confined domains through narrow channels. These phenomena are related to narrow escape problems (NEPs), where one needs to calculate the average time required by an object to escape from or enter the confinement through a small opening. In this project, we perform computer simulations to explore the escape dynamics of a self-propelled (active) nanorod from circular confinements with narrow opening(s). Our results clearly demonstrate how the persistent and directed motion of the nanorod helps it to escape. To quantify the dynamics, we compute the radial probability density function (RPDF) and mean escape time (MFET) and show how the activity is responsible for the bimodality of RPDF, which is clearly absent if the nanorod is passive. The computed mean first escape time decreases with activity. In contrast, the fluctuations of FETs vary in a non-monotonic way. This results in high values of the coefficient of variation and indicates the presence of multiple timescales in first escape time distributions and multimodality in uniformity index distributions.

- **Motility-induced phase separation in presence of obstacles**
  Motility-induced phase separation (MIPS) refers to a phenomenon observed in active matter systems, where self-propelled particles or organisms undergo phase separation unlike conventional phase separation driven by attractive forces. Examples include biological systems (such as bacterial colonies, cell migration, and aggregation), active colloidal suspensions, and even artificial systems like self-propelled robots. It has implications in diverse fields, including soft matter physics, biophysics, materials science, and active matter robotics, providing insights into the dynamics and organization of self-propelled entities. In crowded and complex environments, the presence of obstacles can significantly impact the dynamics of active matter systems. These obstacles can influence the phase separation behavior, leading to spatially varying cluster sizes, shapes, or dynamics. As a result, the interplay between self-propulsion and obstacles can give rise to interesting phenomena in MIPS.

EXPERIENCE AND SKILLS

- Experienced in supervising both undergrads and postgrads.
- 5 years of experience handling simulation packages LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) and Gaussian.

- Self-motivated programmer, experienced in FORTRAN Programming language.
- Knowledge of Shell Scripting and C language.
- Some Experimental Techniques during M.Sc. and Ph.D. Course work.
- Work experience on utilities like OVITO, VMD, Packmol, Moltemplate, Origin, Gnuplot, LaTeX, MATLAB, Gaussian 09, GaussView, Avogadro, Xmgrace, etc.
- Miscellaneous: Experience in Linux and Windows operating systems.

Awards and Fellowships

I have been honored to receive several awards and fellowships that have recognized my academic achievements and potential for research excellence. These include:

- Institute Postdoctoral Fellowship (2023-) issued by Indian Institute of Technology Bombay, India.
- Junior Research Fellowship (2017-2019) awarded by University Grants Commission (UGC), Govt. of India, selected through the Council of Scientific & Industrial Research CSIR-UGC all-India Examination.
- Senior Research Fellowship (2019-2022) issued by University Grants Commission (UGC), Govt. of India, on the basis of research progress.
- Qualified Graduate Aptitude Test in Engineering (GATE 2017), organized by Indian Institute of Technology (IIT) Roorkee on behalf of NCB-GATE for Department of Higher Education, MHRD.
- Qualified Joint Admission Test for Masters (JAM 2015), all-India level online entrance exam conducted by the Indian Institute of Technology (IITs).
- INSPIRE Scholarship during my B.Sc. (2012-2015) and M.Sc. (2015-2017) studies, awarded by the Department of Science and Technology (DST) under the Ministry of Science and Technology, Indian Government.
  This scholarship is awarded to exceptional students who have obtained top 1% aggregate marks in their Class XII examination from any State/Central Education Board, to support their pursuit of higher education.
- Qualified Joint Entrance Examination (JEE 2013), all India entrance examination conducted for the admissions into the Engineering courses.

Teaching Experience

- Teaching Assistant for the undergraduate course *Physical Chemistry* (CH107), IIT Bombay (three times).
- Teaching Assistant for the graduate course *Chemical Bond and Molecular Geometry* (CH425), IIT Bombay.
- Teaching Assistant for the course *Computational Chemistry* (CH504), IIT Bombay.

Mentorship

- M.Sc. project students: Kailash Sahu (2021), Mahesh Kumar (2019), and Himanshu Kumar (2022).
- NIUS Summer/Winter project students: Ajesh Saviour Paravila (2018), and Rohit Raj (2020).

Conference & Workshop

- Workshop on *Advances in Material Science and Material Engineering sponsored by TEQIP-II* at Department of Chemistry, NIT Jalandhar, 08-14 August 2016.
- Poster presentation in *In House Symposium*, Department of Chemistry, IIT Bombay, India, 2020.
- Poster presentation in *Complex Fluids Symposium*, IIT Bombay and the Indian Society of Rheology, India, 2020.
- Poster resentation in *American Physical Society (APS) March Meeting*, 2021.
- Poster presentation in *Duke Soft Matter Symposium*, 2021.
- Poster presentation in *Theoretical Chemistry Symposium*, Indian, 2021.
- Poster presentation in the *Current Trends in Theoretical Chemistry (CTTC-2021)*, Bhabha Atomic Research Centre, India, September 2021.
- Poster presentation in *8TH INDIAN STATISTICAL PHYSICS COMMUNITY MEETING* ICTS Bengaluru, India, 2023.

Position of Responsibilities

- Active member in the organizing team of *Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC8)*, IIT Bombay, Mumbai, India, December 15-17, 2017.

- Volunteer in *Symposium In Memory of Professor Mihir Chowdhury*, IIT Bombay, Mumbai, India, August 2017.

Extracurricular Activities

- Marathon, Cycling, Gym, Sports, and Chess.
- “Roll of Honor” award for outstanding performance and exemplary contribution towards Hostel 13 (House of Titans) as an athlete from 2018 to 2022, IIT Bombay.
- “Best Athlete” award from the Department of Chemistry, IIT Bombay, 2018-2019.
- “Gold Medal” in 5000m Boys Athletic GC from the Department of Chemistry, IIT Bombay, 2018-2019.
- “Gold Medal” in PG CROSSY GC from the Department of Chemistry, IIT Bombay, 2018-2019.
- Participated in “TATA MUMBAI MARATHON” the distance (42.195km) is completed within 3:39:55 hours, 20 January 2019.
- “Sports Special Mention” for outstanding performance and exemplary contribution towards Hostel 13 (House of Titans), IIT Bombay, 2018-2019.
- “Winner of RUNATHON 2019” award for covering a distance of 43.6km within 4 hours, “Institute Record Holder” IIT Bombay, 16 March 2019.

References

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