Curriculum Vitae

Brief Profile:

I am Dr. Projesh Kumar Roy, currently an Assistant Professor in the Department of Chemistry at the National Institute of Technology, Tiruchirappalli. My research expertise lies in the field of Computational and Theoretical Chemistry, with a focus on glasses, polymers, and proteins. I have a deep commitment to advancing scientific understanding through computational techniques, which allow me to probe the intricate molecular details of complex systems. I completed my B.Sc. (Hons.) in Chemistry from Presidency College, University of Calcutta, in 2011. My academic journey continued with my ranking 12^{th} in the IIT-JAM exam, securing a place at the prestigious Indian Institute of Technology, Kanpur, where I earned my M.Sc. in Chemistry in 2013. During this period, I also qualified for both NET (2012) and GATE (2013) exams. Subsequently, I was awarded a competitive doctoral fellowship from the NRW Graduate School of Chemistry, Germany, where I pursued my Ph.D. at the University of Münster.

During my Ph.D., I focused on the structure formation of two-dimensional (2D) silica, a novel allotrope of silica, and developed a Yukawa-based force field that accurately reproduced its key structural properties. My research led to an interesting discovery: the role of an effective temperature factor in driving structure formation, a concept not previously understood under equilibrium conditions. This work opened new avenues for understanding the structure of network glasses and contributed significantly to the field of 2D materials. Following my Ph.D., I undertook post-doctoral research at several renowned institutions. My first post-doctoral position was at the Indian Institute of Science, Bangalore, sponsored by Shell India, where I studied polyimide-based polymeric membranes with applications in gas separation for the oil and natural gas industry. I unraveled the gas adsorption mechanisms at an atomistic level, providing a detailed understanding of how monomer structures influence pore formation in the melt phase. My research extended to gas adsorption studies in dendrimers and carbon molecular sieves, further enhancing our understanding of membrane-based gas separation. At the Institute of Mathematical Sciences, Chennai, I explored the glassy properties of ring polymers, demonstrating that these polymers can form a unique phase known as topological glass under specific conditions of pressure and stiffness. My research also uncovered intriguing phase separation behaviors in topological glasses, adding a new dimension to the study of polymeric materials. In addition, I independently developed a theoretical model based on classical fractional exclusion statistics, a hybrid of classical and quantum statistics. This model has shown promise in explaining exclusion mechanisms in classical systems, and I have applied it to activated molecular dynamics with successful results. Most recently, as a SERB-National Post-Doctoral Fellow at IIT Madras, I have been investigating the mechanism of mutant p53-p73 aggregation, a critical process in cancer biology. My ongoing work aims to design small molecule inhibitors that can disrupt this aggregation and induce apoptosis via the p73 signaling pathway, potentially contributing to cancer treatment.

National Institute of Technology, Tiruchirappalli:
Performa for CV of Faculty/ Staff Members

1. Name: Dr. Projesh Kumar Roy
2. Designation: Assistant Professor
3. Office Address: CH314, OJAS Building, Department of Chemistry.
4. Telephone (Direct) (Optional):

   Telephone: Extn (Optional):

   Mobile (Optional): +91-8583837127
5. Email (Primary): projesh@nitt.edu Email (Secondary): projesh.roy@gmail.com
6. Field(s) of Specialization: Computational Chemistry and Computational Biology.

7. Employment Profile

Job Title	Employer	From	To
Ph. D. Scholar	WWU Münster, Germany	01.10.2013	31.10.2018
Research Associate	IISc, Bangalore	01.01.2019	28.02.2020
Post-Doctoral Fellow	IMSc, Chennai	01.04.2020	30.10.2022
National Post-Doctoral Fellow	IIT-Madras	01.12.2022	31.03.2024

8. Academic Qualifications (From Highest Degree to High School):

Examination	Board / University	Year	Division/ Grade	Subjects
Ph. D.	WWU Münster, Germany	2018	Magna cum Laude	Computational Chemistry
M. Sc.	IIT-Kanpur	2013	1st	Chemistry
B. Sc.	Presidency College, University of Calcutta	2011	1st	Chemistry (Hons.)
H.S.	Bhatpara Amarkrishna Pathsala, WBCHSE	2008	1st	Physics, Chemistry, Mathematics, Biology

9. Academic/Administrative Responsibilities within the University

Position	Faculty/Department/Centre/Institution	From	To
Assistant Professor	Chemistry	02.04.2024	Present
Member of Anti-Ragging Committee	NITT	19.08.2024	19.09.2024

Member of Seating and Logistics Committee (Convocation)	NITT	03.08.2024	03.08.2024

10. Academic/Administrative Responsibilities outside the University

Position	Institution	From	To
M.Sc. supervisor	CIPET: IPT Kochi	Nov 2024	April 2025

11. Awards, Associateships, etc.

Year of Award	Name of the Award	Awarding Organization
2022	SERB-NPDF fellowship	DST-SERB
2013	Ph.D. fellowship	NRW Graduate School of Chemistry, Germany

12. Fellowships

Year of Award	Name of the Fellowship	Awarding Organization	From (Month/Year)	To (Month/Year)
2022	SERB-NPDF fellowship	DST-SERB	01.12.2022	30.11.2024
2020	IPDF fellowship	IMSc, Chennai	01.04.2020	30.11.2022
2013	Ph. D. fellowship	NRW Graduate School of Chemistry	01.10.2013	31.10.2018

13. Details of Academic Work

(i) Curriculum Development:

a. course curriculum for the B.Sc.-B.Ed. program (Physical Chemistry).
b. PG course development CH 624 Multiscale Simulation Methods.

(ii) Courses taught at Postgraduate and Undergraduate levels:

a. PG: CH-629 Polymer Chemistry (2024), CH-631 Electronic structure methods for molecular and solid-state systems (2024)
b. UG: CHIR-11 Chemistry Theory (2024), CHIR-12 Chemistry Practical (2024)

(iii)Projects guided at the Postgraduate level

a. "Understanding the relationship between porosity and structural properties of a coarse-grained polymer model using molecular dynamics technique" – Mr. Anand Venugopal (ongoing)
b. "Understanding thermal resistivity of organic polymers with applications in thermoelectric materials using computational tools" – Mr. Vignesh P N (ongoing)

(iv)Other contribution(s)

14. Details of Major R&D Projects

Title of Project	Funding Agency	Duration		Status
		From	To	Ongoing/ Completed
Unraveling the mechanism of mutant p53-p73 interactions: Useful insights for rational drug design against cancer using computational tools	DST-SERB	01.12.2022	31.11.2024	Ongoing

15. Number of PhDs guided

Name of the PhD Scholar	Title of PhD Thesis	Role(Supervisor/ Co-Supervisor)	Year of Award

16. Participation in Workshops/ Symposia/ Conferences/ Colloquia /Seminars/ Schools etc. (mentioning the role)

Date (s)	Title of Activity	Level of Event (International/ National/ Local)	Role (Participant/ Speaker/ Chairperson, Paper presenter, Any other)	Event Organized by	Venue
20/12/2023	CompFlu 2023	International (within India)	Poster presentation	Indian Society of Rheology, Indian Institute of Technology Madras	Indian Institute of Technology Madras
08/12/2023	Theoretical Chemistry Symposium 2023	International (within India)	Poster presentation	Indian Institute of Technology Madras	Indian Institute of Technology Madras
27/10/2023	Structure and Dynamics of Chemical and Biomolecular Systems 2023	International (within India)	Poster presentation	Indian Institute of Technology Kanpur	Indian Institute of Technology Kanpur
21/12/2022	CompFlu 2022	International (within India)	Poster presentation	Indian Society of Rheology, Indian Institute of Technology Kharagpur	Indian Institute of Technology Kharagpur

02/08/2022	Conference on Computational Physics 2022	International (Abroad)	Seminar	IUPAP	Online
17/07/2022	WE-Heraeus Seminar: Entropy and the second law of thermodynamics	International (Abroad)	Poster presentation	DPG	DPG Bad-Honnef
28/06/2022	EUTOPIA's summer school	International (Abroad)	Poster presentation	University of Paris-City	University of Paris-City
20/03/2022	StatPhysXI	International (within India)	Poster presentation	IISER-Kolkata	IISER-Kolkata
06/01/2021	Digital workshop on glasses	International (Abroad)	Poster presentation	CECAM	CECAM
22/08/2020	RACMS International conference	International (within India)	Seminar	Indian Chemical Society	Indian Chemical Society
27/02/2020	WISCOM 2020	University	Seminar	Holy-cross college, Trichy	Holy-cross college, Trichy
21/02/2020	MolSim Symposium	International (within India)	Poster presentation	Indian Institute of Technology Kanpur	Indian Institute of Technology Kanpur
13/07/2019	Summer school on Rare Events	International (within India)	Poster presentation	Indian Institute of Science, Bangalore	Indian Institute of Science, Bangalore
10/03/2016	DPG Spring Meeting Regensburg	International (Abroad)	Seminar	DPG, Germany	Regensburg
19/03/2015	DPG Spring Meeting Berlin	International (Abroad)	Poster presentation	DPG, Germany	Berlin
01/04/2014	DPG Spring Meeting Dresden	International (Abroad)	Poster presentation	DPG, Germany	Dresden

17. Workshops/ Symposia/ Conferences/ Colloquia/Seminars Organized (as Chairman/ Organizing Secretary/ Convenor / Co-Convenor)

Title of Activity	Level of Event (International/ National/ Local)	Date (s)	Role	Venue

18. Invited Talks delivered

Topic	Date	Inviting Organization
Modelling two-dimensional silica: how does correlation affect the small system thermodynamics?	04.12.2018	Indian Institute of Science, Bangalore
The thermodynamical properties of the random networks in 2D-silica glass	16.12.2019	Institute of Mathematical Sciences Chennai
Basics of Molecular Dynamics Simulation	27.02.2020	Holy Cross College Trichy

19. Membership of Learned Societies

Type of Membership (Ordinary Member/ Honorary Member / Life Member)	Organization	Membership No. with date

20. Academic Foreign Visits

Country	Duration of Visit	Programme
France	27.06.22-12.07.22	EUTOPIA summer school
Germany	13.07.22-19.07.22	WE-Heraeus Seminar: Entropy and the second law of thermodynamics

21. Publications

(A) Refereed Research Journals:

Author(s)	Title of Paper	Journal	Volume (No.)	Page numbers	Year	Impact Factor of the Journal (Optional)
P. K. Roy, M. Heyde, and A. Heuer	Modeling the atomic arrangement of amorphous 2D silica: a network analysis	Physical Chemistry Chemical Physics	20	14725	2018	3.676
P. K. Roy and A. Heuer	Ring Statistics in 2D-silica: Effective Temperatures in Equilibrium	Physical Review Letters	122	016104	2019	8.6

P. K. Roy and A. Heuer	Relating local structures, energies, and occurrence probabilities in a two-dimensional silica network	Journal of Physics: Condensed Matter	31	225703	2019	2.7
P. K. Roy, K. Kumar, F. M. Thakkar, A. D. Pathak, K. G. Ayappa and P. K. Maiti	Investigations on 6FDA/BPDA-DAM polymer melt properties and CO_2 adsorption using molecular dynamics simulations	Journal of Membrane Science	631	118377	2020	9.5
S. Kunalan, K. Dey, P. K. Roy, V. Velachi, P. K. Maiti, K. Palanivelu, and N. Jayaraman	Efficient Facilitated Transport PETIM Dendrimer-PVA-PEG/PTFE Composite Flat-Bed Membranes for Selective Removal of CO_2	Journal of Membrane Science	622	119007	2020	9.5
P. K. Roy, P. Chaudhuri, and S. Vemparala	Effect of ring stiffness and ambient pressure on the dynamical slowdown in ring polymers	Soft Matter	18	2959	2022	3.4
P. K. Roy	Derivation of a statistical model for classical systems obeying fractional exclusion principle	Physical Review E	106	014141	2022	2.4
S. Dasgupta, Rajasekaran M., P. K. Roy, F. M. Thakkar, A. D. Pathak, K. G. Ayappa, and P. K. Maiti	Influence of Polymer Chain Length on Structural Properties of Carbon Molecular Sieving Membranes and Their Effects on CO_2, CH_4 and N_2 Adsorption: A Molecular Simulation Study	Journal of Membrane Science	664	121044	2022	9.5
P. K. Roy, and A. Heuer	Influence of the coordination defects on the dynamics and the potential energy	Journal of Chemical Physics	157	174506	2022	4.4

	landscape of two-dimensional Silica					
P. K. Roy, P. Chaudhuri, and S. Vemparala	Bidisperse ring polymers: topological glass to stacking	Physical Review Materials	8	045601	2024	3.1

(B) Conferences/Workshops/Symposia Proceedings

Author(s)	Title of Abstract/ Paper	Title of the Proceedings	Page numbers	Conference Theme	Venue	Year

(C) Books & Monographs

Author(s)	Title of Book/Monograph	Name of Publishers	Year of Publication	ISSN/ISBN Number