

Dr. Shashi Kumar

Assistant Professor

Department of Chemical Engineering

National Institute of Technology

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EDUCATION

PhD	Department of Chemical Engineering Indian Institute of Technology Kharagpur, India <i>Advisor: Prof. Parag A. Deshpande</i> Thesis title: Computational analysis of thermostability of SazCA	2022
M.Tech	Department of Chemical Engineering Indian Institute of Technology (ISM) Dhanbad, India <i>Advisor: Prof. Souvik Kumar Bhaumik</i> Thesis title: Minimizing axial dispersion in narrow packed column using superhydrophobic wall	2016

RESEARCH EXPERIENCE

Post-Doc	Georgia State University, Atlanta, United States <i>PI: Prof. Iyaylo Ivanov</i> Cryo EM, Molecular Simulations, ML, Protein engineering	June 2023-July 2024
Post-Doc	Computer Aided Drug Design Center University of Maryland, Baltimore, United States <i>PI: Prof. Alex MacKerell</i> Target Drug Delivery, SILCS, Protein Engineering	June 2022-June 2023
PhD	Indian Institute of Technology Kharagpur, India <i>PI: Prof. Parag A. Deshpande</i> Biomolecular simulations, QM/MM Machine Learning, DFT	July 2016-June 2022

M.Tech.	Indian Institute of Technology (ISM) Dhanbad, India <i>PI: Prof. Souvik Kumar Bhaumik</i> Microfluidics: Slip Enhanced Flow and dispersion studies in Packed Column with Thin Superhydrophobic Wall	July 2014-May 2016
B.Tech.	CSIR-Indian Institute of Petroleum, Dehradun, India <i>PI: Dr. Thallada Bhaskar</i> Biofuels, Biomass conversion, Pyrolysis Prepared Micro porous Silica Based catalysts for Biomass Conversion	June 2012-December 2012

SKILL & INTERESTS

- Technical language: TCL, Fortran (basic), Python (Basic)
- Operating systems: Linux, CentOS, Fedora, Windows (XP/10/7)
- Software Packages : NAMD, OpenMM, Gaussian 09, Gaussview, VMD, CryoDRGN, Chimera
- Equipment knowledge : Particle size analyzer, UV-spectroscopy, Contact angle goniometer, HPLC, FTIR, GC
- Interests: Playing Volleyball, Badminton, Running, Listening to music

AREA OF INTERESTS

- Biomolecular simluations, Protein engineering for CCUS processes, Molecular biology, Machine learning, Target drug delivery, Microfluidics, Chemical reaction engineering, QM/MM

PUBLICATIONS

10. **Shashi Kumar**, Soumya Biswas and Parag A. Deshpande, GLY100ALA site point mutation modulates SazCA thermostability, *Journal of Biomolecular Dynamics and Simulation* 1-9.

9. **Shashi Kumar**, Vibhuti Singhania, Vinay Kumar Duggineni and Parag A. Deshpande, Unravelling the factors governing protein thermostability by machine learning, *Advanced Theory and Simulation* 2200703.
8. **Shashi Kumar**, N. Subrahmanyeswara Rao, K.S.S.V. Prasad Reddy, Manjusha C. Padole and Parag A. Deshpande, Enzyme-substrate interactions in orotate-mimetic OPRT inhibitor complexes: A QM/MM analysis, *Physical Chemistry and Chemical Physics* 25(4), 3472-3484.
7. **Shashi Kumar**, and Parag A. Deshpande, Efficient proton shuttle makes SazCA an excellent CO₂ hydration enzyme, *Journal of Biomolecular Structure and Dynamics* 1-10.
6. **Shashi Kumar** and Parag A. Deshpande, Structural and thermodynamic analysis of factors governing the stability and thermal folding/unfolding of SazCA, *PLOS One*, 2021, 6(4):e0249866.
5. Manju Verma, Vangala Sai Phani Kumar, **Shashi Kumar** and Parag A. Deshpande, Biomimetic CO₂ hydration activity of boronic acids, *Physical Chemistry Chemical Physics*, 2021, 23(15), 9561-9570.
4. **Shashi Kumar**, Deepak Seth, and Parag A. Deshpande, Molecular dynamics simulations identify the regions of compromised thermostability in SazCA, *Proteins: Struct. Funct. Bioinf.*, 2021, 89, 375-388.
3. T. Saha, **Shashi Kumar** and Souvik K. Bhaumik, Slip-enhanced flow through thin packed column with superhydrophobic wall, *Sensors and Actuators B: Chemical*, 2017, 240, 468-476.
2. T. Saha, **Shashi Kumar** and Souvik K. Bhaumik, Minimizing axial dispersion in narrow

packed column using superhydrophobic wall, *Korean Journal of Chemical Engineering*, 2016, 33(12), 3337-3342.

1. Rawel Singh, Aditya Prakash, **Shashi Kumar**, Bhavya Balagurumurthy, Ajay K Arora, SK Puri and Thallada Bhaskar, Hydrothermal conversion of lignin to substituted phenols and aromatic ethers, *Bioresource Technology*, 2014, 165, 319-322.

PUBLICATIONS IN CONFERENCE PROCEEDINGS

- 12 articles in conference proceedings (international/national)
- 12 poster presentations (international/national)
- 01 invited talk at MGU, Kottayam
- *h*-index: 6 & citations: 258

SIGNIFICANT OUTREACH ACTIVITIES

- Reviewed journal articles of Materials Today: Proceedings

TEACHING ASSISTANTSHIP EXPERIENCE

Monitoring the experiments conducted by the bachelor and master students

- Teaching Assistant (TA), Chemical Engineering Department, IIT Kharagpur
 - Process Dynamics and Control lab (03 session)
 - Fluid Flow lab (01 session)
 - Chemical reaction engineering in lab (02 session)
- Teaching Assistant (TA), Chemical Engineering Department, IIT (ISM) Dhanbad
 - Instrumental and analysis lab (01 session)
 - Advanced chemical engineering lab (01 session)

GRANTS & HONOURS

- Travel grant from IIT Kharagpur for full financial assistance for American Chemical Society ACS Fall National Meeting & Exhibition 2019 at San Diego, CA, USA.
- Travel grant from IIT Kharagpur for 71th Annual Session of Indian Institute of Chemical Engineers, CHEMCON 2018, NIT, Jalandhar, Punjab, India.
- Scholarship from Ministry of Human Resource Development (MHRD) for PhD in Chemical Engineering.
- University Ranker (2009-2013) in Chemical Engineering.
- Award of Honour as Mukhiya Mantri Protsahan Yojna from Himchal Pradesh Government for carrying out post-graduate studies in IITs at master and PhD level.
- Best poster award for poster presentation at MGU (ICRM-2012), Kottayam, Kerla.
- Best oral presentation award at Science Technical Event at SBSSTC 2013.
- Frist Prize for Quiz contest held at SBSSTC 2012.
- One of the best presentation of sessions award for oral presentation in CHEMCON 2018 at NIT Jalandhar.
- Appreciation certificates for presenting working models, paper and posters in various international and national conferences, university level science Exhibitions and participation in various quiz, declamation contests, painting and in sports.

PROFESSIONAL MEMBERSHIPS

- Member of American Chemical Society (ACS).
 - Life-time member of IChE (Indian Institute of Chemical Engineers).
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POSITION OF RESPONSIBILITY

- Conducted a TEQIP sponsored short term course on Heterogeneous Catalysis for Chemical Engineers, November 10-14, 2018, Department of Chemical Engineering, IIT Kharagpur.
 - Reviewer for Manav Human Atlas Database : a collaborative program of DBT, MHRD and Persistent limited for Human Maps.
 - M.Tech. coordinator at Department of Chemical Engineering, Indian Institute of Technology (ISM) Dhanbad, India.
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References

- Prof. Parag A. Deshpande: Professor, Department of Chemical Engineering, Indian Institute of Technology Kharagpur, India.
Email: parag@che.iitkgp.ac.in
 - Prof. Dr. Thallada Bhaskar: Chief Scientist & HoD, MRED, CSIR-Indian Institute of Petroleum Dehradun, India.
Email: tbhaskar@iip.res.in
 - Prof. Alex MacKerell, Grollman-Glick Professor of Pharmaceutical Sciences
Director, Computer-Aided Drug Design Center, School of Pharmacy,
University of Maryland, Baltimore.
Email: alex@outerbanks.umaryland.edu
 - Prof. Sabyashachi Mishra: Associate Professor, Department of Chemistry, Indian Institute of Technology Kharagpur, India.
Email: sabyashachi.mishra@gmail.com
 - Prof. Debasis Sarkar: Associate Professor, Department of Chemical Engineering, Indian Institute of Technology Kharagpur, India.
Email: dsarkar@che.iitkgp.ac.in
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LINGUISTIC PROFICIENCY

- English (Read, Write and Speak)
- Hindi (Read, Write and Speak)

PROFESSIONAL LINKS

- Google Scholar: <https://scholar.google.co.in/citations?user=kYkZT3sAAAAJ&hl=en>
- ResearchGate: <https://www.researchgate.net/profile/Shashi-Kumar-30>
- LinkedIn: <https://www.linkedin.com/in/dr-shashi-kumar-19b46b57/>
- ORCID: <https://orcid.org/0000-0002-3703-4488>
- SCOPUS: <https://www.scopus.com/authid/detail.uri?authorId=57209548014>
- Researcher ID: <https://www.webofscience.com/wos/author/record/IUP-5607-2023>

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