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Education

Ph. D. Department of Chemical Engineering,
(August 2007 - March 2011) Indian Institute of Science, Bangalore 560012, India
Thesis: Development of ionic catalysts for the
water-gas shift reaction and exhaust gas purification
Adviser: Prof. Giridhar Madras

Bachelor of Engineering Chemical Engineering (with Honours)
(2003-2007) Pt. Ravishankar Shukla University,
Raipur 492001, India

Positions

Associate professor Department of Chemical Engineering,
(March 2018, continuing) Indian Institute of Technology Kharagpur

Assistant professor Department of Chemical Engineering,
(June 2014 - February 2018) Indian Institute of Technology Kharagpur

Assistant professor (tenure track) Department of Chemical Engineering,
(June 2012 - June 2014) Indian Institute of Technology Kharagpur

Postdoctoral fellow Department of Chemical and Biological Engineering,
(April 2011-May 2012) Northwestern University, USA

Fellowships and awards

- DAAD exchange of faculty fellowship 2015
- DST Fast-Track scheme for young scientists (2013-2016)
- India-Austria collaborative research grant 2013-14
- N. R. Kuloor medal for best Ph. D. thesis in the Department of Chemical Engineering, Indian Institute of Science, Bangalore.

- Recipient of *Bristol-Myers Squibb* fellowship offered by Bristol-Myers Squibb, USA (2009-2011).

- University gold medal for chemical engineering for undergraduate degree (2007).

Sponsored projects

1. Topic: *In silico* mechanistic investigations of *de novo* synthesis of *Mycobacterium Tuberculosis* DNA.
PI: P. A. Deshpande
Co-PI: None
Amount: 5,00,000
Funding agency: ISIRD, SRIC, Indian Institute of Technology Kharagpur
Duration: 2013-2016
2. Topic: Analysis of doped oxide catalysts for pharmaceutical reactions.
PI: P. A. Deshpande
Co-PI: None
Amount: 24,00,000
Funding agency: Fast Track Scheme for Young Scientists of Department of Science and Technology, Government of India
Duration: 2013-2016
3. Topic: *In silico* structural and functional investigations of isozymes of carbonic anhydrase family.
PI: P. A. Deshpande
Co-PI: None
Amount: 36,00,000
Funding agency: Department of Biotechnology, Government of India
Duration: 2013-2018
4. Topic: Experimental and theoretical investigations of polymerization-grade ethylene synthesis.
PI: P. A. Deshpande
Co-PI: Dr. Sudhanshu Sharma, Department of Chemistry, IIT Gandhinagar
Co-PI: Dr. Debasis Sarkar, Department of Chemical Engineering, IIT Kharagpur
Amount: 55,00,000
Funding agency: Department of Science and Technology, Government of India
Duration: 2013-2016
5. Topic: Investigation of Suzuki-Miyaura reactions catalyzed by ionic Pd immobilized in inorganic oxide matrix.
PI: P. A. Deshpande
Co-PI: Dr. Heidrun Gruber-Wölfler, Institut für Prozess- und Partikeltechnik, TU Graz, Austria
Amount: INR 8,00,000 + €6,000

Funding agency: India-Austria Scientific-Technological Co-operation 2013-2014, Department of Science and Technology, Government of India
Duration: 2013-2015

6. Topic: Particle engineering by model-based control of ultrasound assisted crystallization processes for organic chemicals and pharmaceuticals.
PI: Dr. Debasis Sarkar, Department of Chemical Engineering, IIT Kharagpur
Co-PI: P. A. Deshpande Amount: INR 37,00,000
Funding agency: Department of Science and Technology, Government of India
Duration: 2016-2019
7. Topic: Development of nanoporous geopolymeric catalysts for industrially relevant liquid-phase reactions.
PI: P. A. Deshpande
Co-PI: Dr. Sudhanshu Sharma, Department of Chemistry, IIT Gandhinagar
Amount: 60,00,000
Funding agency: Department of Science and Technology, Government of India
Duration: 2018-2021

Research supervision (towards doctoral degree)

1. Mr. N. Nagasubrahmanyeswara Rao (January 2013 - December 2017)
Research topic: Studies on mechanistic insights into *Mycobacterium Tuberculosis* DNA by QM/MM calculations.
2. Ms. Manju Verma (January 2013 - May 2018)
Research topic: DFT studies for development of biomimetic heterogeneous catalysts for CO₂ hydration.
3. Ms. Manjusha Padole (January 2014 - September 2017)
Research topic: Studies on adsorption and reactions on doped oxide surfaces using DFT calculations.
4. Mr. P. Phanikumar (January 2015 onwards)
Research topic: DFT insights into structures and functions of ceria-based multicomponent catalysts.
5. Mr. V. Sai Phani Kumar (January 2015 onwards)
Research topic: DFT studies on structure-property relationships of TiO₂-based catalysts.
6. Mr. K. S. S. V. Prasad Reddy (July 2016 onwards)
Research topic: DFT studies on catalysis by transition metal clusters.
7. Mr. Shashi Kumar (July 2016 onwards)
Research topic: Studies on mechanistic insights into carbonic anhydrase action using QM/MM calculations.

8. Mr. Anant Paswan (July 2017 onwards)
Research topic: DFT insights into structure and spectroscopy of surface intermediates over ceria-based catalysts.
9. Ms. Saroj Kumari (July 2017 onwards)
Research topic: Computational analysis of transition metals as CO₂ hydration catalysts.
10. Ms. Swayam Prabha Misra (July 2018 onwards)
Research topic: Computational analysis of geopolymeric catalysts for organic synthesis.

Invited lectures/session chair

1. *Multicomponent nanocrystalline oxide catalysts: Synthesis, characterization and molecular modeling*. Mahatma Gandhi University, Kottayam, Kerala, India, 2014.
2. Session chair, *International Conference on Nanomaterials and Nanocomposites 2014*
3. *Python-based Process Simulations*, National Institute of Technology Raipur, 2014.

Courses taught

1. Advanced mathematical techniques in Chemical Engineering (CH61015; Autumn 2016, Autumn 2017, Autumn 2018)
2. Advanced heat transfer (CH61014; Spring 2019)
3. Chemical engineering thermodynamics (CH21008; Spring 2013, Spring 2014, Spring 2015, Spring 2016, Spring 2017, Spring 2018)
4. Advanced thermodynamics (CH62015; Autumn 2013, Autumn 2014, Autumn 2018)
5. Methods in molecular simulations (TS70001; Spring 2014, Spring 2015)
6. Quantum methods in molecular simulations (TS62002; new course designed for Centre for Theoretical Studies for institute's micro-specialization initiative; Spring 2018, Spring 2019)
7. Science of living systems (BS20001; Autumn 2014, Spring 2015)
8. Chemical reaction engineering laboratory (CH49015; Autumn 2012, Autumn 2013, Autumn 2014, Autumn 2015, Autumn 2016; Autumn 2017)
9. Fluid flow laboratory and design (CH29006; Spring 2013, Spring 2014)
10. Instrumentation and process control laboratory (CH39020; Spring 2013, Spring 2017, Spring 2018, Spring 2019)
11. M. Tech. Design (CH69004; Spring 2014, Spring 2015, Spring 2016, Spring 2017, Spring 2018, Spring 2019)

Short-term courses organized

1. An AICTE-QIP sponsored short term course on *Numerical Techniques of Chemical Process Simulations*, November 20-26, 2017, Department of Chemical Engineering, IIT Kharagpur (jointly with Professor D. Sarkar, Department of Chemical Engineering, IIT Kharagpur)
2. A TEQIP sponsored short term course on *Heterogeneous Catalysis for Chemical Engineers*, November 10-14, 2018, Department of Chemical Engineering, IIT Kharagpur (Co-instructor, jointly with Professor S. Sengupta, Department of Chemical Engineering, IIT Kharagpur)

Academic administration and services

1. Vice-chairperson, Career Development Centre, IIT Kharagpur (January 2017 onwards).
2. Chairman, Purchase committee, Career Development Centre, IIT Kharagpur (2018-19).
3. Member, Academic committee, Centre for Computational Data Sciences, IIT Kharagpur (April 2017 onwards).
4. Member, Hospitality committee, Convocation 2016, 2017, 2018.
5. Member, Technical core committee for development of central high-performance computing facility, IIT Kharagpur.
6. Member, Syllabus review and reformulation committee, Biosciences, IIT Kharagpur.
7. Research scholar coordinator, Department of Chemical Engineering, IIT Kharagpur (June 2016 - June 2017).
8. Member, Faculty search committee, Department of Chemical Engineering, IIT Kharagpur (January 2014 onwards).
9. Member, Infrastructure development committee, Department of Chemical Engineering, IIT Kharagpur (January 2014 - December 2017).
10. Member, Departmental research committee, Department of Chemical Engineering, IIT Kharagpur (January 2014 - December 2017).
11. Member, Departmental purchase committee, Department of Chemical Engineering, IIT Kharagpur (January 2018 onwards).
12. Member, Departmental academic committee, Department of Chemical Engineering, IIT Kharagpur (January 2018 onwards).
13. Member, Departmental academic committee, Centre for Theoretical Studies, IIT Kharagpur (April 2015 onwards).
14. Member, Committee for visitor's programme, Centre for Theoretical Studies, IIT Kharagpur (April 2015 onwards).

15. Professor-in-charge, Training and Placements, Department of Chemical Engineering, IIT Kharagpur (January 2014 - December 2017).
16. Professor-in-charge, Computer Aided Process Engineering Laboratory, Department of Chemical Engineering, IIT Kharagpur (January 2014 onwards).
17. Professor-in-charge, Departmental server administration, Department of Chemical Engineering, IIT Kharagpur (January 2014 onwards).
18. Professor-in-charge, Chemical Engineering Association, IIT Kharagpur (January 2014 onwards - December 2017).

Areas of interest

- Biomimesis: Understanding biochemical systems using quantum chemical calculations and development of analogous chemical systems, particularly for catalytic applications.

- Understanding and development of chemical and biochemical systems of importance in pharmaceutical engineering and chemistry.

- Computational surface science: Computational surface science and its use in catalysis and catalyst design.

Publications

1. Bisht, A., Phanikumar, P., Deshpande, P.A., Sharma, S. $\text{La}_{0.80}\text{Sr}_{0.20}\text{CoO}_3$ as a noble metal-free catalyst for the direct Oxidation of formic acid under zero applied potential (2019) *Electrochemistry Communications*, Article in press.
2. Phani Kumar, V.S., Deshpande, P.A. DFT reveals concentration-dependent cathodic/anodic behaviour of lithiated titania (2018) *Materials Research Express*, 5, pp. 096301.
3. Rao, N.N.S., Deshpande, P.A. QM/MM reveals the sequence of substrate binding during OPRT action (2018) *Computational Biology and Chemistry*, 74, pp. 80-85.
4. Rao, N.N.S., Deshpande, P.A. QM/MM analysis of effect of divalent metal ions on OPRT action (2018) *Computational Biology and Chemistry*, 74, pp. 31-38.
5. Phani Kumar, V.S., Deshpande, P.A. Computational insights into crystal plane dependence of thermal and photoresponse of pure and palladium-substituted titania (2018) *Computational Materials Science*, 143, pp. 528-541.
6. Nayak, A.K., Verma, M., Sohn, Y., Deshpande, P. A., Pradhan, D. Highly active tungsten oxide nanoplate electrocatalysts for the hydrogen evolution reaction in acidic and near neutral electrolytes (2017) *ACS Omega*, 2, pp. 7039-7047.
7. Phani Kumar, V.S., Arya, R., Deshpande, P.A. Computational insights into crystal plane dependence of thermal activity of anion (C and N)-substituted titania (2017) *Physical Chemistry Chemical Physics*, 19, pp. 31452-31460.

8. Verma, M., Deshpande, P.A. Computational insights into biomimetic CO₂ hydration activities of (poly)borate ions (2017) *Journal of Physical Chemistry C*, 121, pp. 17197-17206.
9. Palode, M.C., Deshpande, P.A. Adsorption of C₂ gases over CeO₂-based catalysts: Synergism of cationic sites and anionic vacancies (2017) *Physical Chemistry Chemical Physics*, 19, pp. 14148-14159.
10. Jadhav, D.A., Deshpande, P.A., Ghangrekar, M.M. Enhancing performance of single-chambered microbial fuel cell using manganese/palladium and zirconium/palladium composite cathode catalysts (2017) *Bioresource Technology*, 238, pp. 568-574.
11. Palode, M.C., Deshpande, P.A. Mechanistic insights into C-C cross coupling activities of Pd/Ni-doped heterofullerenes (2017) *Journal of Physical Organic Chemistry*, Article in Press.
12. Verma, M., Deshpande, P.A. Mechanistic insights into biomimetic carbonic anhydrase action catalyzed by doped carbon nanotube and graphene (2017) *Physical Chemistry Chemical Physics*, 19, pp. 8757-8767.
13. Lichtenegger, G.J., Maier, M., Hackl, M., Khinast, J.G., Gossler, W., Griesser, T., Kumar, V.S.P., Gruber-Woelfler, H., Deshpande, P.A. Suzuki-Miyaura coupling reactions using novel metal oxide supported ionic palladium catalysts (2017) *Journal of Molecular Catalysis A: Chemical*, 426, pp. 39-51.
14. Padole, M.C., Deshpande, P.A. Halobenzene activation by heterofullerenes: Computational investigation of oxidative addition activity (2017) *Journal of Physical Organic Chemistry*, 30 (cover article).
15. Palode, M.C., Deshpande, P.A. Acid-base interactions in halobenzene-Ceria systems: Insights into oxidative addition from theory (2016) *Journal of Physical Chemistry C*, 120 (44), pp. 25436-25444.
16. Verma, M., Deshpande, P.A. Computational design of new heterofullerene-based biomimetic α -Carbonic anhydrase analogues (2016) *ChemPhysChem*, pp. 3120-3128.
17. Sharma, S., Sravan Kumar, K.B., Chandnani, Y.M., Phani Kumar, V.S., Gangwar, B.P., Singhal, A., Deshpande, P.A. Mechanistic insights into CO₂ methanation over Ru-substituted CeO₂ (2016) *Journal of Physical Chemistry C*, 120 (26), pp. 14101-14112.
18. Padole, M.C., Deshpande, P.A. Tailoring surface adsorption and reactivity of fullerene-based compounds: A theoretical probe into C₂-gas-fullerene surface interactions (2016) *Journal of Physical Chemistry C*, 120 (23), pp. 12654-12665.
19. Deshpande, P.A. Computational investigation of Cu₇ as a model biomimetic CO₂ capture catalyst (2016) *Chemical Engineering Science*, 145, pp. 294-298.
20. Deshpande, P.A. Nonlinear-to-linear elastic transition in C₆₀ fullerene (2016) *Computational Materials Science*, 115, pp. 117-119.

21. Banerjee, S., Deshpande, P.A. On origin and evolution of carbonic anhydrase isozymes: A phylogenetic analysis from whole-enzyme to active site (2016) *Computational Biology and Chemistry*, 61, pp. 121-129.
22. Verma, M., Sravan Kumar, K.B., Deshpande, P.A. Computational insights into the activity of transition metals for biomimetic CO₂ hydration (2016) *Journal of Physical Chemistry C*, 120 (10), pp. 5577-5584.
23. Rao, N.N.S., Deshpande, P.A. A mechanistic model for uridine 5'-monophosphate nucleotide synthesis (2015) *Chemical Engineering Science*, 134, pp. 504-509.
24. Sravan Kumar, K.B., Deshpande, P.A. On identification of labile oxygen in ceria-based solid solutions: Which oxygen leaves the lattice? (2015) *Journal of Physical Chemistry C*, 119 (16), pp. 8692-8702.
25. Subrahmanyeswara Rao, N.N., Deshpande, P.A. An organism-independent unified model for activity of orotate phosphoribosyltransferases for orotidine monophosphate synthesis (2015) *Chemical Engineering Science*, 128, pp. 109-118.
26. Deshpande, P.A., Poliseti, S., Madras, G., Jyothi, D., Chandrasekaran, S. Dispersed ZrO₂ nanoparticles in MCM-48 with high adsorption activity (2012) *AIChE Journal*, 58 (10), pp. 2987-2996.
27. Deshpande, P.A., Poliseti, S., Madras, G. Analysis of oxide and vanadate supports for catalytic hydrogen combustion: Kinetic and mechanistic investigations (2012) *AIChE Journal*, 58 (3), pp. 932-945.
28. Jyothi, D., Deshpande, P.A., Venugopal, B.R., Chandrasekaran, S., Madras, G. Transition metal oxide loaded MCM catalysts for photocatalytic degradation of dyes (2012) *Journal of Chemical Sciences*, 124 (2), pp. 385-393.
29. Poliseti, S., Deshpande, P.A., Madras, G. Photocatalytic activity of combustion synthesized ZrO₂ and ZrO₂-TiO₂ mixed oxides (2011) *Industrial and Engineering Chemistry Research*, 50 (23), pp. 12915-12924.
30. Anumol, E.A., Kundu, P., Deshpande, P.A., Madras, G., Ravishankar, N. New insights into selective heterogeneous nucleation of metal nanoparticles on oxides by microwave-assisted reduction: rapid synthesis of high-activity supported catalysts (2011) *ACS Nano*, 5 (10), pp. 8049-8061.
31. Deshpande, P.A., Madras, G. Combustion synthesized vanadia rods for environmental applications (2011) *AIChE Journal*, 57 (8), pp. 2215-2228.
32. Kundu, P., Nethravathi, C., Deshpande, P.A., Rajamathi, M., Madras, G., Ravishankar, N. Ultrafast microwave-assisted route to surfactant-free ultrafine Pt nanoparticles on graphene: Synergistic co-reduction mechanism and high catalytic activity (2011) *Chemistry of Materials*, 23 (11), pp. 2772-2780.
33. Ch, R., Deshpande, P.A., Madras, G. Effect of Zr⁴⁺-ion substitution in CeO₂ on H₂O₂-assisted degradation of orange G (2011) *Catalysis Communications*, 12 (11), pp. 940-945.

34. Deshpande, P.A., Poliseti, S., Madras, G. Rapid synthesis of ultrahigh adsorption capacity zirconia by a solution combustion technique (2011) *Langmuir*, 27 (7), pp. 3578-3587.
35. Kundu, P., Deshpande, P.A., Madras, G., Ravishankar, N. Nanoscale ZnO/CdS heterostructures with engineered interfaces for high photocatalytic activity under solar radiation (2011) *Journal of Materials Chemistry*, 21 (12), pp. 4209-4216.
36. Deshpande, P.A., Jain, D., Madras, G. Kinetics and mechanism for dye degradation with ionic Pd-substituted ceria (2011) *Applied Catalysis A: General*, 395 (1-2), pp. 39-48.
37. Deshpande, P.A., Aruna, S.T., Madras, G. Photocatalytic activity of combustion synthesized nanocrystalline CeAlO₃ (2011) *Clean - Soil, Air, Water*, 39 (3), pp. 259-264.
38. Deshpande, P.A., Madras, G. Noble metal ionic sites for catalytic hydrogen combustion: Spectroscopic insights (2011) *Physical Chemistry Chemical Physics*, 13 (2), pp. 708-718.
39. Deshpande, P.A., Aruna, S.T., Madras, G. CO oxidation by CeO₂-Al₂O₃-CeAlO₃ hybrid oxides (2011) *Catalysis Science and Technology*, 1 (9), pp. 1683-1691.
40. Deshpande, P.A., Madras, G. Photocatalytic degradation of phenol by base metal-substituted orthovanadates (2010) *Chemical Engineering Journal*, 161 (1-2), pp. 136-145.
41. Deshpande, P.A., Madras, G. Catalytic hydrogen combustion for treatment of combustible gases from fuel cell processors (2010) *Applied Catalysis B: Environmental*, 100 (3-4), pp. 481-490.
42. Deshpande, P.A., Madras, G. Support-dependent activity of noble metal substituted oxide catalysts for the water gas shift reaction (2010) *AIChE Journal*, 56 (10), pp. 2662-2676.
43. Mahendra Kumar, S., Deshpande, P.A., Krishna, M., Krupashankara, M.S., Madras, G. Photocatalytic activity of microwave plasma-synthesized TiO₂ nanopowder (2010) *Plasma Chemistry and Plasma Processing*, 30 (4), pp. 461-470.
44. Varma, M.N., Deshpande, P.A., Madras, G. Synthesis of biodiesel in supercritical alcohols and supercritical carbon dioxide (2010) *Fuel*, 89 (7), pp. 1641-1646.
45. Deshpande, P.A., Hegde, M.S., Madras, G. A mechanistic model for the water-gas shift reaction over noble metal substituted ceria (2010) *AIChE Journal*, 56 (5), pp. 1315-1324.
46. Deshpande, P.A., Hegde, M.S., Madras, G. Pd and Pt ions as highly active sites for the water-gas shift reaction over combustion synthesized zirconia and zirconia-modified ceria (2010) *Applied Catalysis B: Environmental*, 96 (1-2), pp. 83-93.
47. Deshpande, P.A., Madras, G. Photocatalytic degradation of dyes over combustion-synthesized Ce_{1-x}Fe_xVO₄ (2010) *Chemical Engineering Journal*, 158 (3), pp. 571-577.

48. Sharma, S., Deshpande, P.A., Hegde, M.S., Madras, G. Nondeactivating nanosized ionic catalysts for water-gas shift reaction (2009) *Industrial and Engineering Chemistry Research*, 48 (14), pp. 6535-6543.
49. Baidya, T., Gupta, A., Deshpandey, P.A., Madras, G., Hegde, M.S. High oxygen storage capacity and high rates of CO oxidation and NO reduction catalytic properties of $\text{Ce}_{1-x}\text{Sn}_x\text{O}_2$ and $\text{Ce}_{0.78}\text{Sn}_{0.2}\text{Pd}_{0.02}\text{O}_{2-\delta}$ (2009) *Journal of Physical Chemistry C*, 113 (10), pp. 4059-4068.
50. Roy, S., Marimuthu, A., Deshpande, P.A., Hegde, M.S., Madras, G. Selective catalytic reduction of NO_x : Mechanistic perspectives on the role of base metal and noble metal ion substitution (2008) *Industrial and Engineering Chemistry Research*, 47 (23), pp. 9240-9247.

Book chapters:

1. Gupta, A., Phani Kumar, V.S., Padole, M.C., Saharia, M., Sravan Kumar, K.B., Deshpande P.A. Ceria-based nanocrystalline oxide catalysts: Synthesis, characterization and applications (2017) *Nanomaterials: Physical, Chemical and Biological Applications*, CRC Press, Book in Production.
2. Deshpande, P.A., Madras, G. Catalytic synthesis of CO free hydrogen (2013) *New and Future Developments in Catalysis*, Elsevier, pp. 223-252.
