Parag A. Deshpande

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Education

Ph. D. (2007 - 2011)	Department of Chemical Engineering, Indian Institute of Science, Bengaluru, India
Bachelor of Engineering (2003 - 2007)	Chemical Engineering (with Honours) Pt. Ravishankar Shukla University, Raipur, India

Positions

11 years of post-Ph.D. experience in academia

Fulbright faculty fellow (2021)	Department of Chemical and Biological Engineering, Northwestern University, Evanston, USA
Associate professor (2018 onwards)	Department of Chemical Engineering, Indian Institute of Technology Kharagpur, India
Assistant professor (2014 - 2018)	Department of Chemical Engineering, Indian Institute of Technology Kharagpur, India
Assistant professor (tenure track) (2012 - 2014)	Department of Chemical Engineering, Indian Institute of Technology Kharagpur, India
Postdoctoral fellow (2011 - 2012)	Department of Chemical and Biological Engineering, Northwestern University, Evanston, USA

Short-term visiting appointments

- Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany, June-July 2019.

- Department of Chemistry, Technische Universitat Berlin, Germany, October-December 2015.

- Institute for Process and Particle Technology, Technische Universitat Graz, Austria, December 2013.

Fellowships and awards

- 2020-2021 Fulbright-Nehru academic and professional excellence fellowship

- DAAD exchange of faculty fellowship 2019

- 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, Bengaluru.

- Bristol-Myers Squibb fellowship for doctoral studies (2009-2011).

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

Sponsored projects

Successfully completed externally funded projects of value ∼2.25 crore INR sponsored by the Department of Biotechnology and the Department of Science and Technology, Government of India. Out of 2.25 crore, projects of value ∼1.85 crore INR were undertaken as the PI of the projects.

1. Topic: *In silico* mechanistic investigations of *de novo* synthesis of *Mycobacterium tuberculosis DNA.*
   Role: Principal investigator
   Amount: INR 5,00,000
   Funding agency: ISIRD, Indian Institute of Technology Kharagpur
   Duration: 2013-2016

2. Topic: *In silico* structural and functional investigations of isozymes of carbonic anhydrase family.
   Role: Principal investigator
   Amount: INR 36,00,000
   Funding agency: Department of Biotechnology, Government of India
   Duration: 2013-2018

3. Topic: Analysis of doped oxide catalysts for pharmaceutical reactions.
   Role: Principal investigator
   Amount: INR 26,00,000
   Funding agency: Fast Track Scheme for Young Scientists of Department of Science and Technology, Government of India
   Duration: 2013-2016

4. Topic: Experimental and theoretical investigations of polymerisation-grade ethylene synthesis.

Role: Principal investigator
Amount: INR 55,00,000
Funding agency: Department of Science and Technology, Government of India
Duration: 2013-2016

5. Topic: Investigation of Suzuki-Miyaura reactions catalysed by ionic Pd immobilised in inorganic oxide matrix.
   Role: Principal investigator
   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 crystallisation processes for organic chemicals and pharmaceuticals.
   Role: Co-principal investigator
   PI: Professor Debasis Sarkar, Department of Chemical Engineering, IIT Kharagpur
   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.
   Role: Principal investigator
   Amount: INR 60,00,000
   Funding agency: Department of Science and Technology, Government of India
   Duration: 2018-2021

Research supervision (towards doctoral degree)
Completed the supervision of 8 doctoral students with the sole supervision of 7 students.

1. Mr. N. Nagasubrahmanyeswara Rao (2013 - 2018)
   Thesis title: *In silico* studies on orotate phosphoribosyltransferase action.

2. Ms. Manju Verma (2013 - 2018)
   Thesis title: Computational analysis of biomimetic catalysts for CO_2 hydration.

3. Ms. Manjusha C. Padole (2014 - 2018)
   Thesis title: Computational studies on interaction of C2-gases and halobenzenes with carbonaceous and oxide surfaces.

4. Mr. Vangala Sai Phani Kumar (2015 - 2020)
   Thesis title: Structure-property relationships in TiO_2-based multicomponent catalysts.

5. Mr. Phanikumar Pentyala (2015 - 2020)
   Thesis title: DFT insights into structures and functions of rare earth oxides.

6. Ms. Ankita Agarwal (2015 - 2022; School of Biosciences; joint-supervision with Professor R. Bahadur)
   Thesis title: Computational analysis and prediction of protein-RNA interactions in human RNA-binding proteins.

7. Mr. Shashi Kumar (2016-2022)
   Thesis title: Computational insights into the thermostability of SazCA.

8. Mr. K. S. S. V. Prasad Reddy (2016-2022)
   Thesis title: Computational analysis of small-atom palladium clusters as Suzuki-Miyaura catalysts.

9. Ms. Saroj Kumari (2017 onwards)
   Research topic: Computational analysis of transition metals as biomimetic CO_2 hydration catalysts.

10. Ms. Swayam Prabha Misra (2018 onwards)
    Research topic: Computational analysis of geopolymeric catalysts for organic reactions.

Invited lectures/seminars/session chairship

1. Invited talk in *Beyond Fossil Fuels: The Future of Alternative Energy Technologies*, organised by Indian Institute of Technology, Banaras Hindu University, 2022.

2. Invited talk in *ChemCatCon 2.0: Mechanistic investigations on heterogeneous processes*, organised by Indian Institute of Technology Gandhinagar, 2022.

3. Expert lecture on *Transition metal cluster catalysis: A new domain in catalysis*, in the Department of Chemical Technology, Laxminarayan Institute of Technology Nagpur, 2021.

4. Expert lecture on *Simultaneous CO_2 capture and CH_4 recovery from shale: A comparison of thermodynamics and kinetics*, in the Department of Chemical Engineering, Motilal Nehru National Institute of Technology Allahabad, 2020.

5. Expert lecture on *Thermodynamics of biomolecular systems: Fundamentals and applications*, in the Department of Biotechnology, Motilal Nehru National Institute of Technology Allahabad, 2020.

6. Invited talk in *ChemCatCon 1.0: Reactions on surfaces* organised by Indian Institute of Technology Gandhinagar, 2020.

7. Invited lectures in a TEQIP short term course on computer methods for chemists organised by Department of Chemistry, Indian Institute of Technology Kharagpur, 2020.

8. Invited lectures in a TEQIP short term course on materials science organised by Women's Engineering College Ajmer, 2019.

9. Invited lectures in a TEQIP short term course on catalysis organised by National Institute of Technology Jalandhar, 2019.

10. Invited talk in *ICNM 2014*, Mahatma Gandhi University Kottayam, India, 2014.

11. Session chair, *International Conference on Nanomaterials and Nanocomposites 2014*.

12. Invited lecture on *Python-based process simulations*, in the Department of Chemical Engineering, National Institute of Technology Raipur, 2014.

Courses taught

1. Advanced mathematical techniques in chemical engineering (CH61015; six times between 2016-2022)

2. Advanced thermodynamics (CH62015; four times between 2013-2022)

3. Process dynamics (CH61016; three times between 2020-2022)

4. Biochemical engineering (CH40001; one time in 2022)

5. Advanced heat transfer (CH61014; one time in 2019)

6. Chemical engineering thermodynamics (CH21008; six times between 2013-2018)

7. Quantum methods in molecular simulations (TS62002; three times between 2018-2022)

8. Methods in molecular simulations (TS70001; two times between 2014-2015)

9. Chemical reaction engineering laboratory (CH49015; five times between 2012-2017)

10. Fluid flow laboratory and design (CH29006; two times between 2013-2014)

11. Instrumentation and process control laboratory (CH39020; seven times between 2013-2022)

12. M. Tech. Design (CH69004; nine times between 2014-2022)

NPTEL courses developed

1. Developed NPTEL-SWAYAM course on *Advanced process dynamics*. The course is a 30 h graduate-level course.

Short-term courses organised

1. An AICTE-QIP sponsored short term course on *Numerical Techniques for Chemical Process Simulations*, November 20-26, 2017, Department of Chemical Engineering, IIT Kharagpur (jointly with Professor D. Sarkar, Department of Chemical Engineering, IIT Kharagpur; principal course coordinator and course instructor).

2. A TEQIP sponsored short term course on *Heterogeneous Catalysis for Chemical Engineers*, November 10-14, 2018, Department of Chemical Engineering, IIT Kharagpur (jointly with Professor S. Sengupta, Department of Chemical Engineering, IIT Kharagpur; course co-coordinator and course instructor).

Academic administration and professional services

1. Academic Editor, PLOS ONE.
2. Vice-chairperson, Career Development Centre, IIT Kharagpur (for four placement sessions between 2017-2020).
3. Chairman, Purchase committee, Career Development Centre, IIT Kharagpur (2018-20).
4. Member, Academic committee, Centre for Computational and Data Sciences, IIT Kharagpur.
5. Member, HPC advisory committee, IIT Kharagpur.
6. Member, Technical core committee for development of central high-performance computing facility, IIT Kharagpur.
7. Associate, Centre of Theoretical Studies, IIT Kharagpur (2014-2020).
8. Member, Syllabus review and reformulation committee, Biosciences, IIT Kharagpur.
9. Research scholar coordinator, Department of Chemical Engineering, IIT Kharagpur (2016-2017).
10. Member, Faculty search committee, Department of Chemical Engineering, IIT Kharagpur (2014-2020).
11. Member, Infrastructure development committee, Department of Chemical Engineering, IIT Kharagpur (2014-2017).
12. Member, Departmental administrative committee, Department of Chemical Engineering, IIT Kharagpur (2022 onwards).
13. Member, Departmental research committee, Department of Chemical Engineering, IIT Kharagpur (2014-2017).
14. Member, Departmental purchase committee, Department of Chemical Engineering, IIT Kharagpur (2014 onwards).
15. Member, Departmental academic committee, Department of Chemical Engineering, IIT Kharagpur (2014-2020).
16. Member, Departmental academic committee, Centre for Theoretical Studies, IIT Kharagpur (2015-2020).
17. Member, Committee for visitor's programme, Centre for Theoretical Studies, IIT Kharagpur (2015-2019).
18. Professor-in-charge, Training and Placements, Department of Chemical Engineering, IIT Kharagpur (2014-2017).

19. Professor-in-charge, Computer Aided Process Engineering Laboratory, Department of Chemical Engineering, IIT Kharagpur (2014-2022).

20. Professor-in-charge, Departmental server administration, Department of Chemical Engineering, IIT Kharagpur (2014 onwards).

21. Professor-in-charge, Chemical Engineering Association, IIT Kharagpur (2014-2017).

22. Professor-in-charge, Departmental research facility, Department of Chemical Engineering, IIT Kharagpur (2022 onwards).

23. Member, advisory committee, 2^{nd} National Conference on Advances in Chemical and Environmental Engineering, March 23-24, 2019, National Institute of Technology Jalandhar.

24. Member, publication committee, International Conference on Chemical, Bio and Environmental Engineering, February 13-14, 2020, National Institute of Technology Jalandhar.

25. Member, Technical advisory committee, NanoSeoul 2021, June 08-10, 2021.

Areas of interest

- Computational molecular biology: Developing molecular understanding of structure-function relationships in biological systems using quantum chemical calculations, classical simulations and machine learning.

- Computational catalysis: Understanding and development of catalytic systems of importance in pharmaceutical engineering and chemistry, biomimetic and geophysical carbon capture, clean energy and environment.

- Computational materials science: Developing structure-property relationships in carbonaceous nanomaterials, geopolymers, transition and rare earth oxides.

Publications

75 publications and 2 book chapters with an h-index of 20 as on July 19, 2022.

1. Kumar, S., Deshpande, P.A. Efficient proton shuttle makes SazCA an excellent CO_2 hydration enzyme (2022) Journal of Biomolecular Structure and Dynamics, Article in press.

2. Yadav, P.K., Kumari, S., Uppari, N., Deshpande, P.A., Sharma, S. Insights into the substitutional chemistry of $La_{1-x}Sr_xCo_{1-y}M_yO_3$ (M = Pd, Ru, Rh, and Pt) probed by *in situ* DRIFTS and DFT analysis of CO oxidation (2022) Applied Catalysis A: General, Article in press.

3. Pentyala, P., Deshpande, P.A. Insights into the pathway selectivity during anodic formic acid oxidation over $La_{1-x}Sr_xCoO_3$ (2022) Industrial and Engineering Chemistry Research, Article in press.

4. Prasad Reddy, K.S.S.V., Deshpande, P.A. DFT + U analysis of the stability of $Pd_n/CeO_{2-\delta}$ (n = 3, 4) (2022) Applied Surface Science, Article in press.

5. Prasad Reddy, K.S.S.V., Deshpande, P.A. DFT Reveals the Support Effects in Pd Nanoclusters over Defect-ridden Graphene for the Oxidative Addition of Bromobenzene (2022) Molecular Catalysis, Article in press.

6. Pentyala, P., Singhania, V., Duggineni, V., Deshpande, P.A. Machine learning-assisted DFT reveals key descriptors governing the vacancy formation energy in Pd-substituted multicomponent ceria (2022) Molecular Catalysis, Article in press.

7. Roy, N., Kumari, S., Harshit, Jana, P.P., Deshpande, P.A. Hydrogen storage properties of hexagonal C14 Laves phase Cu_2Cd: A DFT study (2021) Journal of Solid State Chemistry, 304, pp. 122560.

8. Prasad Reddy, K.S.S.V., Deshpande, P.A. Density functional theory study of the immobilisation and hindered surface migration of Pd_3 and Pd_4 nanoclusters over defect-ridden graphene: Implications for heterogeneous catalysis (2021) ACS Applied Nano Materials, 4, pp. 9068-9079.

9. Kumari, S., Deshpande, P.A. OH and O mediated interaction of CO_2 with Ni(110) surface, and its implications on biomimetic CO_2 hydration (2021) Chemical Engineering Science, 246, pp. 116872.

10. Kumar, S., Deshpande, P.A. Structural and thermodynamic analysis of factors governing the stability and thermal folding/unfolding of SazCA (2021) PLOS ONE, 16, pp. e0249866.

11. Pentyala, P., Mohapatra, P.B., Deshpande, P.A. Computational analysis of feasibility of methane displacement by carbon dioxide during enhanced gas recovery from calcite-rich shale (2021) Chemical Engineering Science, 239, pp. 116605.

12. Verma, M., Phani Kumar, V.S., Kumar, S., Deshpande, P.A. Biomimetic CO_2 hydration activity of boronic acids (2021) Physical Chemistry Chemical Physics, 23, pp. 9561-9570.

13. Verma, M., Bhaduri, G.A., Phani Kumar, V.S., Deshpande, P.A. Biomimetic catalysis of CO_2 hydration: A materials perspective (2021) Industrial and Engineering Chemistry Research, 13, pp. 4777-4793 (cover article).

14. Padole, M.C., Kotkar, S.B., Deshpande, P.A. Torsion induced topological deformations in C_{60} (2021) Materials Today Communications, 27, pp. 102201.

15. Roy, N., Kumari, S., Sikdar, R., Sharma, A., Harshit, Ghanta, S., Sharma, S., Deshpande, P.A., Jana, P.P. Synthesis, crystal structure, electronic structure and catalytic properties of Ni_3GaSb (2021) European Journal of Inorganic Chemistry, 14, pp. 1410-1418.

16. Sethulakshmi, N., Nellaiappan, S., Pentyala, P., Sharma, M., Irusta, S., Deshpande, P.A., Sharma, S. Nanocoral $CuCo_2S_4$ thiospinels: Oxygen evolution reaction via redox interaction of metal ions (2021) Electrochimica Acta, 370, pp. 137701.

17. Kumar, S., Seth, D., Deshpande, P.A. Molecular dynamics simulations identify the regions of compromized thermostability in SazCA (2021) PROTEINS, 89, pp. 375-388.

18. Verma, M., Deshpande, P.A. Mechanistic insights into biomimetic CO_2 hydration activity of titania nanoclusters (2021) International Journal of Chemical Kinetics, 2, pp. 265-273.

19. Prasad Reddy, K.S.S.V., Deshpande, P.A. On ligand-free palladium cluster catalysed Suzuki-Miyaura reaction (2020) Physical Chemistry Chemical Physics, 22, pp. 25021-25031.

20. Phani Kumar, V.S., Deshpande, P.A. On interaction of selected biomolecules with a nano-TiO_2 cluster (2020) Computational Biology and Chemistry, 86, pp. 107236.

21. Phani Kumar, V.S., Deshpande, P.A. On Stability of hydroxyl groups on substituted titania (2020) Physical Chemistry Chemical Physics, 22, pp. 1250-1257.

22. Gangwar, B.P., Pentyala, P., Tiwari, K., Biswas, K., Sharma, S., Deshpande, P.A. Dry reforming activity due to ionic Ru in $La_{1.99}Ru_{0.01}O_3$: Role of specific carbonates (2019) Physical Chemistry Chemical Physics, 21, pp. 16726-16736.

23. Pentyala, P., Deshpande, P.A. CO oxidation over $Ce_{1-x}Pd_xO_{2-\delta}$ takes place via vacancy hopping (2019) Industrial and Engineering Chemistry Research, 58, pp. 7964-7972.

24. Phani Kumar, V.S., Deshpande, P.A. Synergistic effect of metal-nonmetal substitution on oxygen activation in Pd/C- and Pd/N-substituted TiO_2 (2019) Computational Materials Science, 162, pp. 349-358.

25. Padole, M.C., Deshpande, P.A. Structural and electronic properties of chemically modified fullerenes (2019) Molecular Simulation, 45, pp. 623-635.

26. Bisht, A., Pentyala, P., Deshpande, P.A., Sharma, S. $La_{0.80}Sr_{0.20}CoO_3$ as a noble metal-free catalyst for the direct Oxidation of formic acid under zero applied potential (2019) Electrochemistry Communications, 99, pp. 1-4.

27. Phani Kumar, V.S., Deshpande, P.A. DFT reveals concentration-dependent cathodic/anodic behaviour of lithiated titania (2018) Materials Research Express, 5, pp. 096301.

28. 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.

29. 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.

30. 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.

31. 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.

32. 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.

33. Verma, M., Deshpande, P.A. Computational insights into biomimetic CO_2 hydration activities of (poly)borate ions (2017) Journal of Physical Chemistry C, 121, pp. 17197-17206.

34. Padole, M.C., Deshpande, P.A. Adsorption of C_2 gases over CeO_2-based catalysts: Synergism of cationic sites and anionic vacancies (2017) Physical Chemistry Chemical Physics, 19, pp. 14148-14159.

35. 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.

36. Padole, M.C., Deshpande, P.A. Mechanistic insights into C-C cross coupling activities of Pd/Ni-doped heterofullerenes (2017) Journal of Physical Organic Chemistry, 30:e3696.

37. 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.

38. 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.

39. Padole, M.C., Deshpande, P.A. Halobenzene activation by heterofullerenes: Computational investigation of oxidative addition activity (2017) Journal of Physical Organic Chemistry, 30:e3628 (cover article).

40. Padole, 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.

41. Verma, M., Deshpande, P.A. Computational design of new heterofullerene-based biomimetic α-Carbonic anhydrase analogues (2016) ChemPhysChem, pp. 3120-3128.

42. Sharma, S., Sravan Kumar, K.B., Chandnani, Y.M., Phani Kumar, V.S., Gangwar, B.P., Singhal, A., Deshpande, P.A. Mechanistic insights into CO_2 methanation over Ru-substituted CeO_2 (2016) Journal of Physical Chemistry C, 120 (26), pp. 14101-14112.

43. Padole, M.C., Deshpande, P.A. Tailoring surface adsorption and reactivity of fullerene-based compounds: A theoretical probe into C_2-gas-fullerene surface interactions (2016) Journal of Physical Chemistry C, 120 (23), pp. 12654-12665.

44. Deshpande, P.A. Computational investigation of Cu_7 as a model biomimetic CO_2 capture catalyst (2016) Chemical Engineering Science, 145, pp. 294-298.

45. Deshpande, P.A. Nonlinear-to-linear elastic transition in C_{60} fullerene (2016) Computational Materials Science, 115, pp. 117-119.

46. 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.

47. Verma, M., Sravan Kumar, K.B., Deshpande, P.A. Computational insights into the activity of transition metals for biomimetic CO_2 hydration (2016) Journal of Physical Chemistry C, 120 (10), pp. 5577-5584.

48. Rao, N.N.S., Deshpande, P.A. A mechanistic model for uridine 5'-monophosphate nucleotide synthesis (2015) Chemical Engineering Science, 134, pp. 504-509.

49. 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.

50. 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.

51. Deshpande, P.A., Polisetti, S., Madras, G., Jyothi, D., Chandrasekaran, S. Dispersed ZrO_2 nanoparticles in MCM-48 with high adsorption activity (2012) AIChE Journal, 58 (10), pp. 2987-2996.

52. Deshpande, P.A., Polisetti, 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.

53. 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.

54. Polisetti, S., Deshpande, P.A., Madras, G. Photocatalytic activity of combustion synthesized ZrO_2 and ZrO_2-TiO_2 mixed oxides (2011) Industrial and Engineering Chemistry Research, 50 (23), pp. 12915-12924.

55. 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.

56. Deshpande, P.A., Madras, G. Combustion synthesized vanadia rods for environmental applications (2011) AIChE Journal, 57 (8), pp. 2215-2228.

57. 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.

58. Chalamalasetti, R., Deshpande, P.A., Madras, G. Effect of Zr^{4+}-ion substitution in CeO_2 on H_2O_2-assisted degradation of orange G (2011) Catalysis Communications, 12 (11), pp. 940-945.

59. Deshpande, P.A., Polisetti, S., Madras, G. Rapid synthesis of ultrahigh adsorption capacity zirconia by a solution combustion technique (2011) Langmuir, 27 (7), pp. 3578-3587.

60. 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.

61. 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.

62. Deshpande, P.A., Aruna, S.T., Madras, G. Photocatalytic activity of combustion synthesized nanocrystalline $CeAlO_3$ (2011) Clean - Soil, Air, Water, 39 (3), pp. 259-264.

63. 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.

64. Deshpande, P.A., Aruna, S.T., Madras, G. CO oxidation by CeO_2-Al_2O_3-$CeAlO_3$ hybrid oxides (2011) Catalysis Science and Technology, 1 (9), pp. 1683-1691.

65. Deshpande, P.A., Madras, G. Photocatalytic degradation of phenol by base metal-substituted orthovanadates (2010) Chemical Engineering Journal, 161 (1-2), pp. 136-145.

66. 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.

67. 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.

68. Mahendra Kumar, S., Deshpande, P.A., Krishna, M., Krupashankara, M.S., Madras, G. Photocatalytic activity of microwave plasma-synthesized TiO_2 nanopowder (2010) Plasma Chemistry and Plasma Processing, 30 (4), pp. 461-470.

69. 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.

70. 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.

71. 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.

72. Deshpande, P.A., Madras, G. Photocatalytic degradation of dyes over combustion-synthesized $Ce_{1-x}Fe_xVO_4$ (2010) Chemical Engineering Journal, 158 (3), pp. 571-577.

73. 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.

74. Baidya, T., Gupta, A., Deshpande, P.A., Madras, G., Hegde, M.S. High oxygen storage capacity and high rates of CO oxidation and NO reduction catalytic properties of $Ce_{1-x}Sn_xO_2$ and $Ce_{0.78}Sn_{0.2}Pd_{0.02}O_{2-\delta}$ (2009) Journal of Physical Chemistry C, 113 (10), pp. 4059-4068.

75. 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.

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