

FACULTY PROFILE



Name	Dr. Milind M. Deshmukh					Date of Birth: February 05, 1978				
Designation	Assistant Professor			Date of holding Present Post			Nov, 30, 2013			
Name of the Department and School	Department of Chemistry School of Chemical Sciences and Technology									
Contact Details	Email : milind.deshmukh@gmail.com					Mobile:8989180813				
Additional Responsibility in the university, if any	Member of Equal Opportunity Cell In-charge-Computer Laboratory of Department of Chemistry									
Educational Qualifications (UG onwards)	M. Sc. (Physical Chemistry), 2001, University of Pune, Pune Ph. D. (Chemistry): 2008, University of Pune: Supervisor. Professor Shridhar R. Gadre									
Research Area/Specialization	Physical Chemistry, Quantum Chemistry Theoretical and Computational Chemistry,									
Awards/ Honors / Fellowship Conferred (With details thereof)	1. 2015: UGC-Assistant Professor Under Faculty recharge Programme (but Not Availed) 2. 2004: Senior Research Fellowship (SRF) of Council of Scientific & Industrial Research (CSIR) 3. 2006: Extended Senior Research Fellowship (SRF-Extn) of Council of Scientific & Industrial Research (CSIR) 4. 2017: Best Poster Award: International Conference on Interface of Physical, Chemical and Biological Sciences,									
Summary of Publications (Number only)	Research Papers	22	Books	-	Chapter in Books	-	Seminars/ Conferences Proceedings	-	Projects	01
Best Five Research Publications	1. Deshmukh, M. M.; Ohba, M.; Kitagawa, S.; Sakaki S. <i>Absorption of CO₂ and CS₂ into the Hofmann-type porous coordination polymer: electrostatic versus dispersion</i> <i>Journal of the American Chemical Society</i> 2013 , 135, 4840-4849. ISSN: 1520-5126 (Web) Impact Factor: 14.695									
	2. Deshmukh, M. M.; Sakaki S. <i>Generation of dihydrogen molecule and hydrosilylation of carbon dioxide catalyzed by zinc hydride complex: theoretical understanding and prediction.</i> <i>Inorganic Chemistry</i> 2014 , 53, 8485–8493. ISSN: 1520-510X(Web) Impact Factor: 4.850									
	3. Singh, V.; Nakao, Y.; Sakaki S.; Deshmukh, M. M. <i>Theoretical study of nickel catalyzed selective alkenylation of pyridine: Reaction mechanism and crucial roles of Lewis acid and ligands in determining the selectivity.</i> <i>The Journal of Organic Chemistry</i> 2017 , 82, 289-301. ISSN: 1520-6904 (Web) Impact Factor: 4.745									
	4. Singh, V.; Sakaki S.; Deshmukh, M. M. <i>Ni(II)-Hydride Catalyst for Hydrosilylation of Carbon Dioxide and Dihydrogen Generation: Theoretical Prediction and Exploration of Full Catalytic Cycle.</i> <i>Organometallics</i> , 2018 , 37, 1258–1270. ISSN: 1520-6041 (Web) Impact Factor: 4.100									
	5. Deshmukh, M. M.; Gadre, S. R.; Bartolotti, L. J. <i>Estimation of intramolecular hydrogen bond energy via molecular tailoring approach,</i> <i>The Journal of Physical Chemistry A</i> 2006 , 110, 12519-12523 ISSN: 1520-5215 (Web) Impact Factor: 2.641									

Research Projects (Completed and Ongoing):

S.No.	Title	Funding Agency	Duration	Sanction order No. & Date	Amount in Rs.	Completed/ongoing
1.	Catalytic Activation of Dihydrogen and Carbon Dioxide with Heavier Main- Group Elements: Theoretical Exploration of New Catalytic Cycles	UGC-STARTUP	2014-2016	No. F.30-56/2014/BSR	Rs. 6,00,000	Completed

PUBLICATIONS : 22
National Publications (Details of Research Papers): 01

2004	1. Gadre, S. R.; Deshmukh, M. M.; Kalagi, R. P. <i>Quantum chemical investigations on explicit molecular hydration, Proceedings of Indian National Science Academy, 2004, 70A, 709-724</i> ISSN: 2454-9983 (Web) Impact Factor: 0754
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International Publications (Details of Research Papers): 24

2020	2. Singh, V.; Ibnusaud, I.; Gadre S. R.; Deshmukh, M. M. Fragmentation Method Reveals a Wide Spectrum of Intramolecular Hydrogen Bond Energies in Antioxidant Natural Products. <i>New Journal of Chemistry. 2020, 44, 5841-5849</i> ISSN: 1369-9261 (Web) Impact Factor: 3.069
2019	3. Singh, V.; Sakaki S.; Deshmukh, M. M. Theoretical Prediction of Ni(I)-Catalyst for Hydrosilylation of Pyridine and Quinoline. <i>Journal of Computational Chemistry, 2019, 40, 2119-2130.</i> ISSN: 1096-987X (Web) Impact Factor: 3.224
2019	4. Kumar, A.; Hung, C. -H.; Rana, S.; Deshmukh, M. M. Study on the Structure, Stability, and Tautomerisms of meta-Benziporphodimethene and N-Confused Isomers Containing g-Lactam Ring. <i>Journal of Molecular Structure 2019, 1187, 138-150</i> ISSN: 0022-2860 (Web) Impact Factor: 2.120
2018	5. Singh, V.; Sakaki S.; Deshmukh, M. M. Ni(I)-Hydride Catalyst for Hydrosilylation of Carbon Dioxide and Dihydrogen Generation: Theoretical Prediction and Exploration of Full Catalytic Cycle. <i>Organometallics, 2018, 37, 1258-1270.</i> ISSN: 1520-6041 (Web) Impact Factor: 4.100
2017	6. Singh, V.; Nakao, Y.; Sakaki S.; Deshmukh, M. M. Theoretical study of nickel catalyzed selective alkenylation of pyridine: Reaction mechanism and crucial roles of Lewis acid and ligands in determining the selectivity. <i>The Journal of Organic Chemistry 2017, 82, 289-301.</i> ISSN: 1520-6904 (Web) Impact Factor: 4.745
2015	7. Deshmukh, M. M.; Gadre, S. R.; Cocinero, E. M. Stability of conformationally locked free fructose: theoretical and computational insights. <i>New Journal of Chemistry. 2015, 39, 9006-9018.</i> ISSN: 1369-9261 (Web) Impact Factor: 3.069
2015	8. Siddiqui, N.; Singh V.; Deshmukh, M. M.; Gurunath, R. Structures, stability and hydrogen bonding in inositol conformers <i>Physical Chemistry Chemical Physics 2015, 17, 18514-18523.</i> ISSN: 1463-9084 (Web) Impact Factor: 3.567
2014	9. Mishra, B. K.; Deshmukh, M. M.; Ramanathan, V. <i>C-H...π interactions and the nature of the donor carbon atom</i> <i>The Journal of Organic Chemistry 2014, 79, 8599-8606.</i> ISSN: 1520-6904 (Web) Impact Factor: 4.745
2014	10. Deshmukh, M. M.; Sakaki S. Generation of dihydrogen molecule and hydrosilylation of carbon dioxide catalyzed by zinc hydride complex: theoretical understanding and prediction <i>Inorganic Chemistry 2014, 53, 8485-8493.</i> ISSN: 1520-510X(Web) Impact Factor: 4.850

2013	11. 14.Deshmukh, M. M.; Ohba, M.; Kitagawa, S.; Sakaki S. <i>Absorption of CO₂ and CS₂ into the Hofmann-type porous coordination polymer: electrostatic versus dispersion</i> <i>Journal of the American Chemical Society</i> 2013, 135, 4840-4849. ISSN: 1520-5126 (Web) Impact Factor: 14.695
2012	12. Khedkar, J. K.; Deshmukh, M. M.; Gejji, S. P.; Gadre, S. R. <i>Intramolecular hydrogen bonding and cooperative interactions in calix[n]arenes (n=4,5)</i> <i>The Journal of Physical Chemistry A</i> 2012, 116, 3739-3744. ISSN: 1520-5215 (Web) Impact Factor: 2.641 13. Deshmukh, M. M.; Sakaki S. <i>Two-step evaluation of potential energy surface and binding energy of van der Waals complexes,</i> <i>Journal of Computational Chemistry</i> 2012, 33, 617-628. ISSN: 1096-987X (Web) Impact Factor: 3.224
2011	14. Deshmukh, M. M.; Sakaki S. <i>Binding energy of gas molecule with two pyrazine molecules as organic linker in metal-organic framework: its theoretical evaluation and understanding of determining factors</i> <i>Theoretical Chemistry Accounts</i> 2011, 130, 475-482 ISSN: 1432-2234 (Web) Impact Factor: 1.598 15. Deshmukh, M. M.; Bartolotti, L. J.; Gadre, S. R. <i>Intramolecular hydrogen bond energy and cooperative interactions in alpha-, beta-, and gamma-cyclodextrin conformers</i> <i>Journal of Computational Chemistry</i> 2011, 32, 2996-3004 ISSN: 1096-987X (Web) Impact Factor: 3.224
2009	16. Deshmukh, M. M.; Gadre, S. R. <i>Estimation of N-H...O=C intramolecular hydrogen bond energy in polypeptides,</i> <i>The Journal of Physical Chemistry A</i> 2009, 113, 7927-7932 ISSN: 1520-5215 (Web) Impact Factor: 2.641
2008	17. Deshmukh, M. M.; Gadre, S. R.; Tonner, R.; Frenking, G. <i>Molecular electrostatic potential of divalent carbon(0) compounds,</i> <i>Physical Chemistry Chemical Physics</i> 2008, 10, 2298-2301 ISSN: 1463-9084 (Web) Impact Factor: 3.567 18. Deshmukh, M. M.; Bartolotti, L. J.; Gadre, S. R. <i>Intramolecular hydrogen bonding and cooperative interactions in carbohydrates via the molecular tailoring approach</i> <i>The Journal of Physical Chemistry A</i> 2008, 112, 312-321 ISSN: 1520-5215 (Web) Impact Factor: 2.641
2007	19. Deshmukh, M. M.; Suresh, C. H.; Gadre, S. R. <i>Intramolecular hydrogen bond energy in polyhydroxy systems: a critical comparison of molecular tailoring and isodesmic approaches,</i> <i>The Journal of Physical Chemistry A</i> 2007, 111, 6472-6480 ISSN: 1520-5215 (Web) Impact Factor: 2.641
2006	20. Deshmukh, M. M.; Gadre, S. R.; Bartolotti, L. J. <i>Estimation of intramolecular hydrogen bond energy via molecular tailoring approach,</i> <i>The Journal of Physical Chemistry A</i> 2006, 110, 12519-12523 ISSN: 1520-5215 (Web) Impact Factor: 2.641
2004	21. Deshmukh, M. M.; Sastry, N. V.; Gadre, S. R. <i>Molecular interpretation of water structuring and destructuring effects: hydration of alkanediols,</i> <i>The Journal of Chemical Physics</i> 2004, 121, 12402-12402 ISSN: 1089-7690 (Web) Impact Factor: 2.997 22. Gadre, S. R.; Deshmukh, M. M.; Chakraborty, T. <i>Electrostatics-guided ab initio studies on weakly bonded complexes of substituted naphthalenes</i> <i>Chemical Physics Letters</i> 2004, 384, 350-356 ISSN: 0009-2614 (Web) Impact Factor: 1.901

National Seminar/Conference/Workshops (Attended)	
Year (From 2013 to 2020)	(with topic, date and venue)
2019	1. Theoretical Chemistry Symposium, BITS-Pilani, Pilani (February, 2019).
2016	2. Theoretical Chemistry Symposium, Hyderabad University, Hyderabad (December, 2016)
2016	3. Science Fair and National Science Day Celebration, Dr. Harisingh Gour Vishwavidyala, Sagar, (Feb-2016)
2015	4. National Symposium on Horizons of Light Molecules, Material and Daily Life (December 2015)
2009	5. National Conference on Changing Paradigms in Theoretical and Computational Chemistry, Department of Chemistry, University of Pune, (December 2009).
2008	6. 10 th CRSI National Symposium in Chemistry, IISc, Bangalore (February 2008).
2008	7. A Seminar on Advances in Chemistry, University of Pune (March 2008)
2006	8. National Symposium on Computational Chemistry, Thiruvananthapuram (Dec. 2006)
2004	9. Theoretical Chemistry Symposium, BARC, Mumbai (December 2004)
2004	10. A workshop on Molecular Modeling and Pharmainformatics, NIPER, (November, 2004).
2004	11. XXXIII National Seminar on Crystallography, NCL, Pune, (January, 2004).
2002	12. Participated in Workshop on Genetic Algorithm in Bioinformatics, Organized by C-DAC, Pune (August 2002)
2001	13. Participated in Workshop on Ab initio Quantum Chemistry, Organized by C-DAC and Department of Chemistry, University of Pune, Pune (November 2001)
International Seminar/Conference/Workshops (Attended)	
2017	14. International conference on Interface of Physical, Chemical and Biological Sciences organized, Dr. Harisingh Gour University during January 11-13, 2017
2017	15. Asia Pacific Conference in Theoretical and Computational Chemistry (APCTCC8). APCTCC, IIT Bombay (December 2017).
2013	16. RSC Conference: Challenges in Organic Materials & Supramolecular Chemistry (ISACS 10), Kyoto University, Japan (June 18-21, 2013).
2011	17. The 7 th Congress of the "International Society for Theoretical Chemical Physics" (ISTCP-VII) Tokyo, Japan (September 2011)
2011	18. The 9 th Triennial Congress of the "World Association of Theoretical and Computational Chemists" (WATOC 2011) at Santiago de Compostela, Spain (July, 2011).
2011	19. The 14 th Annual Meeting of Theoretical Chemistry Society, Okayama, Japan (May 2011).
2010	20. The 8 th Fukui Institute symposium Kyoto, Japan (December 2010).
National Seminar/Conference/Workshops (Organised)	
Year (From 2013 to 2020)	(with topic, date and venue)
2017	1. Conducted National workshop on conceptual Quantum Chemistry (WCQC-2017) during January 16-20, 2017
2015	2. Member of Treasurer Committee In National Science Day Celebration, 2015, Organized by Dr. Harisingh Gour Vishwavidyalata, Sagar.
2014	3. Member of Treasurer Committee In National Science Day Celebration, 2014, Organized by Dr. Harisingh Gour Vishwavidyalata, Sagar.
International Seminar/Conference/Workshops (Organised)	
2017	4. Member of Technical Organizing Committee. International conference on Interface of Physical, Chemical and Biological Sciences organized, Dr. Harisingh Gour University during January 11-13, 2017
Research Papers in Proceedings (National Seminar/Conference/Workshops)	
Year (From 2013 to 2020)	(with title of the paper, Title of the proceedings vol., name of the publisher, Year, page nos.)
-	NONE
Research Papers in Proceedings (International Seminar/Conference/Workshops)	

Year (From 2013 to 2020)	(with title of the paper, Title of the proceedings vol., name of the publisher, Year, page nos.) NONE	
Invited Lectures delivered (<i>Outside University</i>) with title, date and place:		
2019	Invited Lecture In Theoretical Chemistry Symposium, BITS-Pilani, Pilani (February, 2019). Title: <i>Theoretical Prediction Of Novel Ni(I)-Catalyst For The Hydrosilylation of Pyridine And Quinoline: Exploration Of Full Catalytic Cycle.</i>	
No. of Ph.D. Awarded:		01
No. of Ph.D. Scholars working:		01
No. of Foreign Visits : 02		
Year (From 2013 to 2020)	Name of the country, Date, Place, Purpose of visit, duration, etc.	
2010-2013	Japan, June 2010 to 2013, Kyoto University, Kyoto, Japan, Postdoctoral Research Fellow	
2011	Spain, July 17-22, 2011, Santiago de Compostela, Spain For attending international Conference: The 9 th Triennial Congress of the "World Association of Theoretical and Computational Chemists" (WATOC 2011) .	
Memberships in Academic Bodies:		
Member Royal Society of Chemistry 2013		
Other Academic Achievements :		
(i) Membership of Editorial Boards: National/ International (With details of the journal(s) and duration)		
-NONE-		
(ii) Reviewer of the Journal(s) (With details of the journal(s) and duration)		
2020: ACS Catalysis, 2019: Organometallics , 2018: Journal of Molecular Liquids, 2018: ACS Omega, 2018: <i>The Journal of Physical Chemistry B</i> 2018: AIP Advances, 2018 : Chemistry Select, 2017: Journal of Computational Chemistry 2014: Indian Journal of Chemical Science, 2011: Journal of Computational Chemistry 2011: Journal of Computational Chemistry 2010: Journal of Computational Chemistry	Publisher: American Chemical Society Publisher: American Chemical Society Publisher: Elsevier Publisher: American Chemical Society Publisher: American Chemical Society Publisher: American Institute of Physics Publisher: Wiley-VCH Publisher: Wiley-VCH Publisher: CSIR-NISCAIR Publisher: John Wiley & Sons Publisher: John Wiley & Sons Publisher: John Wiley & Sons	

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