



Dr. Rajendra Prasad

Professor

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PROFESSIONAL EXPERIENCE

Duration	Position & Organization	Teaching/Research Area
Oct22,2015 -Present	Professor	Theoretical & Computational Quantum Chemistry.
Oct22,2009- Oct21,2015	Reader/Associate Professor S G B Amravati University, Amravati	Theoretical & Computational Quantum Chemistry.
Mar 2007- Oct 21,2009	CSIR Scientist pool Department of Chemistry, Banaras Hindu University, Varanasi.	<i>The fermion sign problem</i> in the electronic structure quantum diffusion Monte Carlo simulation.
Aug, 2006- Feb, 2007	Department of Chemistry, Banaras Hindu University, Varanasi.	The electronic structure quantum diffusion Monte Carlo simulations.
Mar, 2005- Jul, 2006	Post Doctoral Researcher Lawrence Berkeley National Laboratory, Berkeley University of California Berkeley,USA	<i>Quantum Monte Carlo:</i> Improvement of trial functions used in the electronic structure quantum diffusion Monte Carlo simulations.
Jul, 2004- Feb, 2005	Post Doctoral Researcher University of California Davis, USA	Excited state electronic structure and properties of heavy metal clusters
Oct, 2001- Feb, 2004	Post Doctoral Researcher Lehrstuhl fuer Theoretische Chemie, Ruhr-Universitaet Bochum, Germany and Department of Chemical Physics, Fritz-Haber Institute, Berlin, Germany.	<i>Surface Science:</i> Stereo dynamics of photodesorbed CO from Cr2O3 (0001) surface, <i>ab-initio</i> embedded quantum cluster calculations were performed to obtain several excited states 4D PES for Cr2O3(0001) surface.

AWARDS & FELLOWSHIPS:

2001	Fast Track Young Scientist Project, Science and Engineering Research Council, New Delhi, India. (Awarded while working abroad therefore not executed).
1997-2000	Senior Research Fellowship (University Grants Commission, India).
1995-1997	Junior Research Fellowship (University Grants Commission, India).
1995	Graduate Aptitude Test in Engineering (GATE)

EDUCATIONAL BACKGROUND:

Jun., 2001 Ph.D.	Banaras Hindu University, Varanasi 221 005, India Doctor of Philosophy in Theoretical & Computational Quantum Chemistry. Title of Thesis: " <i>MRD-CI STUDIES OF ELECTRONIC STRUCTURE AND MOLECULAR PROPERTIES OF TRANSIENT MOLECULES</i> "
Sep., 1994 M.Sc. First Div. (61.3%)	Banaras Hindu University, Varanasi 221 005, India. Major Subjects: Physical and Nuclear Chemistry Minor Subjects: Organic, Inorganic and Analytical Chemistry.
Jun., 1992 B. Sc	Banaras Hindu University, Varanasi 221 005, India. Honors Subject: Chemistry

First Div. (69.0%) Jun., 1988 Intermediate	Subsidiary Subjects: Physics and Mathematics Board of High School and Intermediate Education, Utter Pradesh, India. Queens Inter College, Varanasi.
First Div. (66.4%) July, 1986 High School	Subjects: General Hindi, English, Physics, Chemistry, and Mathematics. Board of High School and Intermediate Education, Utter Pradesh, India. Queens Inter College, Varanasi.
First Div. (72.0%)	Subjects: Hindi, English, Mathematics, Science, Social Science and Biology.

MEMBERSHIP OF PROFESSIONAL BODIES

- Life Member
1. Asia-Pacific Association of Theoretical and Computational Chemists (APATCC)
 2. Indian Science Congress Association (ISCA)

CHAIRMAN/MEMBER OF UNIVERSITY BODIES/COMMITTEES

- Member
- Committee to prepare/write proposal under the scheme Promotion of University Research and Scientific Excellence (PURSE) Grant for Sant Gadge Baba Amravati University.
- Chairman
- Research Advisory Committee, Research Center
Department of Chemistry, Sant Gadge Baba Amravati University.
- Member
- Steering Committee, National Institutional Ranking Framework (NIRF), Sant Gadge Baba Amravati University.
- Chairman
- Committee for the Promotion of Excellence in Teaching and Research in the University Departments, Sant Gadge Baba Amravati University.
- Chairman
- Committee to frame regulations for the Professor Emeritus Scheme, Sant Gadge Baba Amravati University.
- Member
- Committee No. 5/2021 to frame regulations for Checking and Penalizing for plagiarism in Research and Publications, Sant Gadge Baba Amravati University.

Author's (Rajendra Prasad) Research Output Impact Matrices/Citation Report**Author's research outcome (as on 18.09.2021)**

1.	Number of publications in Peer-Reviewed/Refereed Journals	39
2.	Number of publications in the journals indexed in SCOPUS	38
3.	Number of publications in the journals/proceedings indexed in Web of Science	38
4.	Number of publications in the journals indexed in Science Citation Index Expanded(SCIE)	37
5.	Number of publications having Impact Factor (Thomson Reuters)	37
6.	Total sum of the Impact Factor (Thomson Reuters)	131.702
7.	Average Impact Factor (Thomson Reuters)	3.560
8.	Number of publications with impact factor between 0 and 1	2
9.	Number of publications with impact factor between 1 and 2	2
10.	Number of publications with impact factor between 2 and 5	27
11.	Number of publications with impact factor between 5 and 10	6
12.	Number of publications in the JCR best JCR Category Quartile: Q1	16
13.	Number of publications in the JCR best JCR Category Quartile: Q2	10
14.	Number of publications in the JCR best JCR Category Quartile: Q3	7
15.	Number of publications in the JCR best JCR Category Quartile: Q4	4

Author's Research Performance Impact

	Parameter ↓ / Database →	Google Scholar	SCOPUS	Web of Science
1.	No. of documents listed	39	38	37
2.	Sum of times cited	2183	1820	1631
3.	Sum of times cited (excluding self-citations)		1787	1600
4.	Average Citations per Item	56.0	47.9	44.8
5.	Average Citations per Year	109.1	91.0	77.7
6.	h-index	18	17	16
7.	h-index (excluding self-citations)	--	17	16
8.	i10	23	23	22
9.	i20	18	15	15
10.	i25	16	13	13
11.	i30	13	13	13
12.	i40	11	10	9
13.	i50	8	5	6
14.	i100	5	4	4

Journal Impact Information 2021 from Journal Citation Reports (Thomson Reuters)

Journal Titles	JCR Category	Impact Factor 2020	Best Category Quartile	Record Count
Corrosion Science	Materials Science, Multidisciplinary - SCIE	7.205	Q1	3
Dalton Transactions	Chemistry, Inorganic & Nuclear - SCIE	4.390	Q1	2
Spectrochimica Acta Part A	Spectroscopy - SCIE	4.098	Q1	2
CrystEngComm	Crystallography - SCIE	3.545	Q1	3
Journal of Chemical Physics	Physics, Atomic, Molecular & Chemical - SCIE	3.488	Q1	6
Solar Energy	Energy & Fuels - SCIE	5.742	Q2	1
Bulletin of the Chemical Society of Japan	Chemistry, Multidisciplinary - SCIE	5.488	Q2	1
Arabian Journal of Chemistry	Chemistry, Multidisciplinary - SCIE	5.165	Q2	1
Materials Chemistry and Physics	Materials Science, Multidisciplinary - SCIE	4.094	Q2	1
Polyhedron	Chemistry, Inorganic & Nuclear - SCIE	3.052	Q2	1
Inorganica Chimica Acta	Chemistry, Inorganic & Nuclear - SCIE	2.545	Q2	1
Inorganic Chemistry Communications	Chemistry, Inorganic & Nuclear - SCIE	2.495	Q2	1
Chemical Physics	Physics, Atomic, Molecular & Chemical - SCIE	2.348	Q2	2
Chemical Physics Letters	Physics, Atomic, Molecular & Chemical - SCIE	2.328	Q2	1
Journal of Molecular Structure	Chemistry, Physical - SCIE	3.196	Q3	5
Journal of Applied Electrochemistry	Electrochemistry - SCIE	2.800	Q3	1
Journal of Solid State Electrochemistry	Electrochemistry - SCIE	2.647	Q3	1
International Journal of Electrochemical Science	Electrochemistry - SCIE	1.765	Q4	1
Australian Journal of Chemistry	Chemistry, Multidisciplinary - SCIE	1.321	Q4	1
Journal of Theoretical and Computational Chemistry	Chemistry, Multidisciplinary - SCIE	0.939	Q4	1
Indian Journal of Chemistry Section A	Chemistry, Multidisciplinary - SCIE	0.491	Q4	1

RESEARCH, PUBLICATIONS AND ACADEMIC CONTRIBUTIONS.**Published Papers in Journals**

Sr. No.	Author(s), Title. <i>Journal</i> . Volume , pages, (Year). Accepted on Day-Month-Year, Published on Day-Month-Year, ISSN, Publisher, Indexed in the database, Peer Reviewed: YES/NO, Impact Factor (Thomson Reuters) .
1.	R. Prasad, P. Chandra, <i>Ab-initio</i> MRD-CI Studies of electric field gradient (efg) and dipole moment of CCN radical at CASSCF optimized geometries for $X^2\Pi$, $a^4\Sigma^-$, $A^2\Delta$, $B^2\Sigma^-$ and $C^2\Sigma^+$ electronic states. <i>Indian Journal of Chemistry–Section A</i> . 39 , 148–162 (2000). Accepted on 26-Nov-1999, Published on Jan-Mar-2000, ISSN:03764710, Publisher: NISCAIR, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 0.483 .
2.	Rajendra Pd, P. Chandra, Ground and valence excited states of C_2N and CN_2 transients: <i>ab initio</i> geometries, electronic structures, and molecular properties. <i>Journal of Chemical Physics</i> . 114 , 1589–1600 (2001). Accepted on 27-Oct-2000, Published on 10-Jan-2001, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters):3.488 .
3.	Rajendra Pd, P. Chandra, Ground and excited states of HNC, NH, and NH_2 transients: <i>Ab initio</i> geometries, electronic structures, and molecular properties. <i>Journal of Chemical Physics</i> . 114 , 7450–7460 (2001). Accepted on 06-Feb-2001, Published on 19-Apr-2001, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.488 .
4.	R. L. Prasad, R. Prasad, G. C. Bhar, S. N. Thakur, Photoacoustic spectra and modes of vibration of TNT and RDX at CO2 laser wavelengths. <i>Spectrochimica Acta - Part A</i> : 58 , 3093–3102 (2002). Accepted on 18-Jan-2002, Published on 20-Mar-2002, ISSN: 13861425, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 4.098 .
5.	R. Prasad, Theoretical study of fine and hyperfine interactions in N_3^+ , N_3 , and N_3^- . <i>Journal of Chemical Physics</i> . 119 , 9549–9558 (2003). Accepted on 12-Aug-2003, Published on 24-Oct-2003, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.488 .
6.	R. Prasad, A theoretical study of the fine and hyperfine interactions in the NCO and CNO radicals. <i>Journal of Chemical Physics</i> . 120 , 10089–10100 (2004). Accepted on 02-Mar-2004, Published on 11-May-2004, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.488 .
7.	R. Prasad, N. Umezawa, D. Domin, R. Salomon-Ferrer, W. A. Lester Jr, Quantum Monte Carlo study of first-row atoms using transcorrelated variational Monte Carlo trial functions. <i>Journal of Chemical Physics</i> . 126 , art. no. 164109 (2007). Accepted on 16-Feb-2007, Published on 25-Apr-2007, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.488 .

8.	<p>A. Aspuru-Guzik, B. Austin, D. Domin, P. T. A. Galek, N. C. Handy, R. Prasad, R. Salomon-Ferrer, N. Umezawa, and W. A. Lester Jr., Recent developments in quantum Monte Carlo: Methods and applications. <i>AIP Conference Proceedings</i>. 963, 210-211 (2007).</p> <p>Accepted on 26-Dec-2007, Published on 08-Jan-2008, ISSN: 0094243X, Publisher: American Institute of Physics, Indexed in Web of Science (WoS), Peer Reviewed : YES, Impact Factor (Thomson Reuters): No.</p>
9.	<p>N. Singh, R. Prasad, S. Bhattacharya, Structural studies on $\text{Ph}_3\text{MSMPh}_3$ (M = Sn, Pb): Quest for a metal-metal bond. <i>Polyhedron</i>. 28, 548–552 (2009).</p> <p>Accepted on 19-Nov-2008, Published on 02-Jan-2009, ISSN: 02775387, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.052.</p>
10.	<p>S. Jaiswal, A. Kushwaha, R. Prasad, R. L. Prasad, R. A. Yadav, Structural and vibrational studies of molecular conductors using quantum mechanical methods: 1,3-Dithiole-2-thione, 1,3-dithiole-2-one, 1,3-dioxole-2-one and 1,3-dioxole-2-thione. <i>Spectrochimica Acta - Part A</i>: 74, 16–25 (2009).</p> <p>Accepted on 23-Feb-2009, Published on 09-Mar-2009, ISSN: 13861425, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 4.098.</p>
11.	<p>K. K. Upadhyay, S. Upadhyay, K. Kumar, R. Prasad, X-ray crystallographic study of 3-Oxo-2-$\{[4-(\text{thiazol-2-ylsulfamoyl})\text{-phenyl}]\text{-hydrazono}\}$-butyric acid ethyl ester and its application in the solvent assisted naked eye sensing of Hg(II). <i>Journal of Molecular Structure</i>. 927, 60–68 (2009).</p> <p>Accepted on 25-Feb-2009, Published on 06-Mar-2009, ISSN: 00222860, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.196.</p>
12.	<p>K. K. Upadhyay, A. Kumar, R. K. Mishra, R. Prasad, Colorimetric recognition of d^{10} metal ions through an adenine-based ICT probe. <i>Bulletin of the Chemical Society of Japan</i>. 82, 813–815 (2009).</p> <p>Accepted on 25-Mar-2009, Published on 10-Jul-2009, ISSN: 00092673, Publisher: Chemical Society of Japan, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 5.488.</p>
13.	<p>R. L. Prasad, A. Kushwaha, R. Prasad, S. Jaiswal, R. A. Yadav, Energetics and structural insights of molecular conductors using density functional theory methods: 1,3-dithiole-2-thione, 1,3-dithiole-2-one, 1,3-dioxole-2-one, and 1,3-dioxole-2-thione. <i>Journal of Theoretical and Computational Chemistry</i>. 8, 1185–1195 (2009).</p> <p>Accepted on 05-May-2008, Published on 28-Mar-2009, ISSN: 02196336, Publisher: World Scientific (Singapore), Indexed in Science Citation Index Expanded (SCIE), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 0.939.</p>
14.	<p>A. Kumar, R. Prasad, G. Kociok-Köhn, K. C. Molloy, N. Singh, Synthesis, structure and calculated NLO properties of $[(n\text{-Bu})_2\text{Sn}-\mu\text{-O}-\mu\text{-OH-Sn}(n\text{-Bu})_2(\text{CH}_3\text{CO}_2)]_2$ and its putative derivatives. <i>Inorganic Chemistry Communications</i>. 12, 686–690 (2009).</p> <p>Accepted on 23-May-2009, Published on 28-May-2009, ISSN: 13877003, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.495.</p>
15.	<p>S. K. Sen Gupta, R. Prasad, Origin and nature of transmission modes of anomalous effects of meta-Substituents on the ^{13}C chemical shift of the carboxyl carbon (δCO) of benzoic acid. <i>Australian Journal of Chemistry</i>. 63, 321–328 (2010).</p> <p>Accepted on 26-Sep-2009, Published on 26-Feb-2010, ISSN: 00049425, Publisher: CSIRO Publishing (Australia), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 1.321.</p>

16.	<p>K. K. Upadhyay, R. K. Mishra, A. Kumar, J. Zhao, R. Prasad, Self assembled pseudo double helix architecture and anion sensing behavior of a coumarin based ICT probe. <i>Journal of Molecular Structure</i>. 963, 228–233 (2010).</p> <p>Accepted on 22-Oct-2009, Published on 29-Oct-2009, ISSN: 00222860, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.196.</p>
17.	<p>I. Ahamad, R. Prasad, M. A. Quraishi, Thermodynamic, electrochemical and quantum chemical investigation of some Schiff bases as corrosion inhibitors for mild steel in hydrochloric acid solutions. <i>Corrosion Science</i>. 52, 933–942 (2010).</p> <p>Accepted on 07-Nov-2009, Published on 13-Nov-2009, ISSN: 0010938X, Publisher: Pergamon-Elsevier Science Ltd, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 7.205.</p>
18.	<p>N. Singh, A. Kumar, R. Prasad, K. C. Molloy, M. F. Mahon, Syntheses, crystal, photoluminescence and electrochemical investigation of some new phenylmercury(ii) dithiocarbamate complexes involving ferrocene. <i>Dalton Transactions</i>. 39, 2667–2675 (2010).</p> <p>Accepted on 10-Dec-2009, Published on 20-Jan-2010, ISSN: 14779226, Publisher: Royal Society of Chemistry (United Kingdom), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 4.390.</p>
19.	<p>I. Ahamad, R. Prasad, M. A. Quraishi, Adsorption and inhibitive properties of some new Mannich bases of Isatin derivatives on corrosion of mild steel in acidic media. <i>Corrosion Science</i>. 52, 1472–1481 (2010).</p> <p>Accepted on 13-Jan-2010, Published on 20-Jan-2010, ISSN: 0010938X, Publisher: Pergamon-Elsevier Science Ltd, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 7.205.</p>
20.	<p>I. Ahamad, R. Prasad, M. A. Quraishi, Experimental and theoretical investigations of adsorption of fexofenadine at mild steel/hydrochloric acid interface as corrosion inhibitor. <i>Journal of Solid State Electrochemistry</i>. 14, 2095–2105 (2010).</p> <p>Accepted on 02-Mar-2010, Published on 30-Mar-2010, ISSN: 14328488, Publisher: Springer Verlag, Indexed in Science Citation Index Expanded (SCIE), Peer Reviewed : YES, Impact Factor (Thomson Reuters): 2.647.</p>
21.	<p>I. Ahamad, R. Prasad, M. A. Quraishi, Inhibition of mild steel corrosion in acid solution by Pheniramine drug: Experimental and theoretical study. <i>Corrosion Science</i>. 52, 3033–3041 (2010).</p> <p>Accepted on 19-May-2010, Published on 23-May-2010, ISSN: 0010938X, Publisher: Pergamon-Elsevier Science Ltd, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 7.205.</p>
22.	<p>J. Chaturvedi, S. Bhattacharya, R. Prasad, Novel heterobimetallic thiocarboxylato complexes: Synthesis, characterization and application as single source precursor for ternary chalcogenides. <i>Dalton Transactions</i>. 39, 8725–8732 (2010).</p> <p>Accepted on 26-Jun-2010, Published on 16-Aug-2010, ISSN: 14779226, Publisher: Royal Society of Chemistry (United Kingdom), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 4.390.</p>
23.	<p>Ahamad, R. Prasad, M. A. Quraishi, Experimental and quantum chemical characterization of the adsorption of some Schiff base compounds of phthaloyl thiocarbohydrazide on the mild steel in acid solutions. <i>Materials Chemistry and Physics</i>. 124, 1155–1165 (2010).</p> <p>Accepted on 14-Aug-2010, Published on 15-Sep-2010, ISSN: 02540584, Publisher: Elsevier (Taiwan), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 4.094.</p>

24.	<p>I. Ahamad, C. Gupta, R. Prasad, M. A. Quraishi, An experimental and theoretical investigation of adsorption characteristics of a Schiff base compound as corrosion inhibitor at mild steel/hydrochloric acid interface. <i>Journal of Applied Electrochemistry</i>. 40, 2171–2183 (2010).</p> <p>Accepted on 05-Sep-2010, Published on 19-Sep-2010, ISSN: 00201693, Publisher: Springer (Netherlands), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.800.</p>
25.	<p>S. K. Roy, R. Prasad, P. Chandra, Electron correlation and relativistic effects in atomic structure calculations of the thorium atom. <i>Journal of Chemical Physics</i>. 134, art. no. 234302 (2011).</p> <p>Accepted on 18-May-2011, Published on 15-Jun-2011, ISSN: 00219606, Publisher: American Institute of Physics, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.488</p>
26.	<p>V. Singh, A. Kumar, R. Prasad, G. Rajput, M.G.B. Drew and N. Singh, The interplay of secondary Hg...S, Hg...N and Hg...n bonding interactions in supramolecular structures of phenylmercury(ii) dithiocarbamates. <i>CrystEngComm</i>. 13, 6817–6826 (2011).</p> <p>Accepted on 15-Aug-2011, Published on 15-Sep-2011, ISSN: 14668033, Publisher: Royal Society of Chemistry (United Kingdom), Indexed in Science Citation Index (SCI), Peer Reviewed : YES, Impact Factor (Thomson Reuters): 3.545.</p>
27.	<p>A. K. Singh, G. Saxena, R. Prasad, A. Kumar, Synthesis, characterization and calculated non-linear optical properties of two new chalcones. <i>Journal of Molecular Structure</i>. 1017, 26–31 (2012).</p> <p>Accepted on 28-Feb-2012, Published on 12-Mar-2012, ISSN: 00222860, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed : YES, Impact Factor (Thomson Reuters): 3.196.</p>
28.	<p>I. Ahamad, R. Prasad, E. E. Ebenso, M. A. Quraishi, Electrochemical and quantum chemical study of albendazole as corrosion inhibitor for mild steel in hydrochloric acid solution. <i>International Journal of Electrochemical Science</i>. 7, 3436–3452 (2012).</p> <p>Accepted on 03-Mar-2012, Published on 01-Apr-2012, ISSN: 14523981, Publisher: ESG (Belgrade). Indexed in Science Citation Index Expanded (SCIE), Peer Reviewed : YES, Impact Factor (Thomson Reuters): 1.765.</p>
29.	<p>S. Bhadauria, S. Saxena, R. Prasad, P. Sharma, R. Prasad, R. Dwivedi, Synthesis of ethylene carbonate from cyclocondensation of ethylene glycol and urea over ZnO•Cr₂O₃ catalyst system controlled by co-precipitation method. <i>European Journal of Chemistry</i>. 3, 235–240 (2012).</p> <p>Accepted on 08-Mar-2012, Published on 30-Jun-2012, ISSN: 21532249, Publisher: Atlanta Publishing House LLC , Indexed in CrossRef, Peer Reviewed : YES, Impact Factor (Thomson Reuters): No.</p>
30.	<p>S. K. Roy, R. Prasad, S. N. Datta, P. Chandra, Electron correlation and relativistic effects in atomic structure calculations of Th⁺, Th²⁺ ions. <i>Chemical Physics Letters</i>. 550, 25–32 (2012).</p> <p>Accepted on 24-Aug-2012, Published on 13-Sep-2012, ISSN: 00092614, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.328.</p>
31.	<p>S. Yadav, A. Moheman, A. Kumar, R. Prasad, K. S. Siddiqi, Conformational isomers of dichloro bis(1,3-diaminopropane) copper(II): Synthesis, characterization and DFT modeling. <i>Arabian Journal of Chemistry</i>. 10, S1435–S1444 (2017).</p> <p>Accepted on 17-Apr-2013, Published on 25-Apr-2013, ISSN: 18785352, Publisher: Elsevier, Indexed in Science Citation Index Expanded (SCIE), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 5.165.</p>

32.	R. Chauhan, S. Auvinen, A. S. Aditya, M. Trivedi, R. Prasad, M. Alatalo, D. P. Amalnerkar, A. Kumar, Light harvesting properties of ferrocenyl based sensitizer with sulfur rich dithiocarbamates and xanthate as anchoring group. <i>Solar Energy</i> . 108 , 560–569 (2014). Accepted on 06-Aug-2014, Published on 03-Sep-2014, ISSN: 0038092X, Publisher: Pergamon-Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 5.742.
33.	R. Prasad, R. Yadav, M. Trivedi, G. Kociok-Köhn, A. Kumar, The interplay of thiophilic and hydrogen bonding interactions in the supramolecular architecture of phenylmercury 4-hydroxypiperidine dithiocarbamate. <i>Journal of Molecular Structure</i> . 1103 , 265–270 (2016). Accepted on 01-Oct-2015, Published on 09-Oct-2015, ISSN: 00222860, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.196.
34.	R. Yadav, M. Trivedi, G. Kociok-Köhn, R. Prasad, A. Kumar, New Ni(II) 1,2-bis(diphenylphosphino) ethane dithiolates: Crystallographic, computational and Hirshfeld surface analyses. <i>CrystEngComm</i> . 17 , 9175–9184 (2015). Accepted on 23-Oct-2015, Published on 26-Oct-2015, ISSN: 14668033, Publisher: Royal Society of Chemistry (United Kingdom), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.545.
35.	R. Yadav, M. Trivedi, R. Chauhan, R. Prasad, G. Kociok-Köhn, A. Kumar, Supramolecular architecture of organotin(IV) 4-hydroxypiperidine dithiocarbamates: Crystallographic, computational and Hirshfeld surface analyses. <i>Inorganica Chimica Acta</i> . 450 , 57–68 (2016). Accepted on 12-May-2016, Published on 20-May-2016, ISSN: 00201693, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.545.
36.	R. Yadav, M.K. Awasthi, A. Singh, G. Kociok-Köhn, M. Trivedi, R. Prasad, M. Shahid, A. Kumar, Molecular structure, supramolecular association and anion sensing by chlorodiorganotin(IV) methylferrocenyldithiocarbamates. <i>Journal of Molecular Structure</i> . 1145 , 197–203 (2017). Accepted on 24-May-2017, Published on 24-May-2017, ISSN: 00222860, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.196.
37.	J.C. Jin, J. Wu, Y.X. He, B.H. Li, J.Q. Liu, R. Prasad, A. Kumar, and S.R. Batten, A 3D luminescent Zn(II) MOF for the detection of high explosives and the degradation of organic dyes: An experimental and computational study. <i>CrystEngComm</i> . 19 , 6464–6472 (2017). Accepted on 04-Oct-2017, Published on 04-Oct-2017, ISSN: 14668033, Publisher: Royal Society of Chemistry (United Kingdom), Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 3.545.
38.	S. K. Roy, R. Prasad, The multiplet electronic structure of UO^+ ion: Relativistic two-component <i>ab initio</i> approach. <i>Chemical Physics</i> . 523 , 75–82 (2019). Accepted on 16-Apr-2019, Published on 17-Apr-2019, ISSN: 03010104, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.348.
39.	S. K. Roy, R. Prasad, The relativistic all-electron <i>ab initio</i> calculations on the multiplet electronic structure of U^{3+} ion. <i>Chemical Physics</i> . 535 , 110781 (2020). Accepted on 29-Mar-2020, Published on 31-Mar-2020, ISSN: 03010104, Publisher: Elsevier, Indexed in Science Citation Index (SCI), Peer Reviewed: YES, Impact Factor (Thomson Reuters): 2.348.

Sanctioned/Ongoing/Completed Research Projects/Consultancies

Sr. No.	Title	Agency	Period	Grant /Amount Mobilized(Rs. Lakh)
1	"The fermion sign problem in the quantum diffusion monte Carlo simulation" Order No. SR/S2/CMP-0003/2011 dated 05.03.2012*Not executed.	Science & Engineering Research Board (SERB) DST, New Delhi	2012-2015	14.3

Training Courses, Teaching-Learning-Evaluation Technology Programmes, Faculty Development Programmes (not less than one week duration).

Sr. No.	Programme	Duration	Organized by
1.	SERC Winter School on Quantum Chemistry	Three weeks Dec.4-24, 1998	IIT Bombay and NCL Pune, India
2.	European Summer School in Quantum Chemistry (ESQC-01) at Tjörnarp Conference Center, Sweden.	Two weeks Aug.19 – Sep.1, 2001	The University of Lund Sweden

Papers/Posters presented in Conferences, Seminars, Workshops, Symposia

Sr. No.	Title of the Paper Presented	Title of Conference / Seminar	Organized by	Whether international/ national/ state/ regional/ college or university level
1.	<i>Ab initio</i> configuration interaction calculations of electric field gradient at ^{35}Cl and ^2H nuclei in $\text{SiCl}_2(^1A_1)$, SiH_2Cl_2 , SiH_3Cl , and SiHCl_3 : a comparative study with Hartree-Fock SCF	2 nd Conference of the International Academy of Physical Sciences	Guru Ghasidas University, Bilaspur (MP) India on December 13-14, 1997.	International
2.	Poster presentation: Title: <i>Ab initio</i> studies of hyperfine interactions in NCO and CNO transients.	European Summer School in Quantum Chemistry (ESQC-01)	University of Lund, Sweden on Saturday, August 25, 2001.	International
3.	POSTER presentation: Title: Laser induced photodesorption of CO from $\text{Cr}_2\text{O}_3(0001)$ surface	11 th International Congress of Quantum Chemistry.	University of Bonn, Germany on July 20-26, 2003.	International
4.	POSTER presentation: Title: Laser induced photodesorption of CO from $\text{Cr}_2\text{O}_3(0001)$ surface: An <i>ab-initio</i> quantum chemical study	39 th Symposium on Theoretical Chemistry 2003(STC-03): Molecular Spectroscopy and Dynamics.	ETH-Zurich 28 th September to 2 nd October 2003, Gwatt, Lake Thun, Switzerland.	International
5.	POSTER No. PII-53: Title: Diffusion Monte Carlo study of Li-Ne using transcorrelated variational Monte Carlo trial function	The American Conference on Theoretical Chemistry 2005 (ACTC-2005)	University of California, Los Angeles held on July 16-21, 2005	International