




Faculty Details proforma for DU Web-site

Title	Prof.	First Name	Rita	Last Name	Kakkar	
Designation		Professor				
Address		<i>Off.</i> Department of Chemistry, University of Delhi, Delhi-110007. <i>Res.</i> 24/1 Mall Road, Delhi - 110007				
Phone No	Office	27667725 Ext. 1390, 27666646 Ext. 204				
Residence		27666313				
Mobile		9810120508				
Email		ritakakkar10@gmail.com, ritakakkar@yahoo.com, rkakkar@chemistry.du.ac.in				
Educational Qualifications						
Degree	Institution			Year		
Ph.D.	University of Delhi.			1982		
M.Phil.	Department of Chemistry, University of Delhi.			1978		
PG	Chemistry (Physical Chem. Spl.), Miranda House, University of Delhi.			1977		
UG	B.Sc.(Hons.) Chemistry, Department of Chemistry, University of Delhi.			1975		
Career Profile						
Lecturer (20 th October, 1981- 9 th December, 1984), Miranda House, University of Delhi. Lecturer (Dec. 10, 1984-Oct. 19, 1991), Senior Lecturer (Oct.20, 1991-Oct.19, 1994), Reader (Oct. 20, 1994-May 4, 2003), Professor (May 5, 2003 onwards), Department of Chemistry, University of Delhi.						
Administrative Assignments						
Member, UGC Syllabus Committee for Choice Based Credit System. Coordinator, B. Sc. Chemistry Examinations (2010-2012), (2014 onwards) Provost, Undergraduate Hostel for Girls (UGHG), Delhi University (2014 onwards) Provost, North Eastern Students' House for Women (NESHW), Delhi University (2007-2010). Member, Interim Committee on Sexual Harassment, Faculty of Science. Member, Governing Bodies of various colleges of Delhi University. Member, Managing Committee of NESHW (2006-2007) & DU Press. Member, Selection Committees within the University and outside. Convener, Physical Chemistry Section, Department of Chemistry, University of Delhi (2014-15). Convener, Library Committee, Department of Chemistry, University of Delhi (2014- Convener, UV-Vis Instrument Committee, Department of Chemistry (2014- Convener (Anti-Sexual Harassment Committee, Department of Chemistry (2014-						
Areas of Interest / Specialization						
Physical Chemistry, Quantum Chemistry, Spectroscopy, Computational Chemistry, Nanoscience.						
Subjects Taught						

Undergraduate

B.Sc. (Hons.) & General - Thermodynamics, Quantum Chemistry, Spectroscopy, Photochemistry

Postgraduate

Quantum chemistry, Spectroscopy & Diffraction, Statistical Thermodynamics, Kinetics & Macromolecules, Computational Chemistry, Advanced Spectroscopy, Advanced Quantum Chemistry

M.Tech. (Nanoscience & Nanotechnology)

Quantum Mechanics

M.Tech. (Chemical Processing & Technology)

Bioinformatics, Molecular Modelling and Drug Design

M.Phil./Ph.D.

Symmetry in Chemistry, Molecular Spectroscopy, Applications of HMO theory, Computer Programming for Chemists.

Practicals

All B.Sc. (Hons.) & M.Sc. Physical Chemistry

Research Guidance**Supervision of awarded Doctoral Thesis**

35. Gulia, Sunita. 2014. Theoretical studies of bio-conjugated and transition metal doped ZnO quantum dots.

34. Arora, Richa. 2014. *In silico* studies of hydroxamic acids and their biological applications.

33. Malik, Pragati. 2014. Theoretical studies on some quantum dots.

32. Kumari, Tripti. 2014. *In silico* studies of PDF inhibitors. University of Delhi.

31. Issar, Upasana. 2014. Theoretical studies on DNA minor-groove binding agents. University of Delhi (22-10-2009).

30. Tyagi, Jyoti. 2013. Theoretical studies of interaction of inorganic and organic pollutants with graphene. University of Delhi.

29. Kohli, Esha. 2013. DFT studies on urease inhibitors. University of Delhi (11-02-2010).

28. Sharma, Neha. 2013. DFT studies on reactions and decomposition of some chemical and biological warfare agents on mixed metal oxide nanostructures. University of Delhi.

27. Gupta, Shweta. 2012. Synthesis, characterization and application of Langmuir-Blodgett films of noble metals. University of Delhi.

26. Singh, Chayannika. 2012. Interaction of kojic acid with quantum dots and DNA bases: A DFT study. University of Delhi.

25. Umesh Kumar, 2011. Synthesis and characterization of nanostructured semiconducting materials and nanocomposites. University of Delhi.

24. Singh, Jyoti, 2011. Theoretical study of CdSe quantum dots and their interactions. University of

Delhi.

23. Thareja, Rakhi. 2010. Quantum chemistry in action: Applications and properties of II-VI quantum dots. University of Delhi.

22. Gaba, Ritu, 2010. DFT study of nanocrystalline TiO₂: Relationships between size, structure and reactivity. University of Delhi.

21. Gupta, Deepti. 2010. Structural properties of maleic and fumaric acids and catalytic role of metal oxides in their degradation: A DFT study. University of Delhi.

20. Bhandari, Mamta. 2010. The alloxan-dialuric acid system: Insights into the diabetogenic activity of alloxan. University of Delhi.

19. Ojha, Himanshu. 2009. Design and biological evaluation of some 2,4,6-triazine antimalarials- A combined computational and experimental study. University of Delhi.

18. Sharma, Smriti. 2009. Functionalization of carbon and boron nitride nanotubes with carbenes- A density functional study. University of Delhi.

17. Das, Achintya. 2008. Computer simulations of lectin-carbohydrate interactions. University of Delhi.

16. Zaidi, Sheza. 2008. The Curtius and Schmidt reactions: A DFT mechanistic study. University of Delhi.

15. Gahlot, Pragya. 2008. *In silico* studies of protein-ligand interactions of some metabolic enzymes. University of Delhi.

14. Dua, Amita. 2007. Conformations and metal complexes of thiohydroxamic acids: A DFT study. University of Delhi.

13. Pathak, Mallika. 2006. A theoretical study of the structure and unimolecular decomposition pathways of pyruvic acid. University of Delhi.

12. Rajni. 2005. Conformers and metal complexes of hydroxamic acids: A density functional study. University of Delhi.

11. Chadha, Preeti. 2005. Density Functional study of some carbene rearrangements. University of Delhi.

10. Suruchi. 2003. Computational studies on the design of radioprotectors based on the Hoechst family. University of Delhi.

9. Garg, Ritu. 2001. Theoretical Studies on modification of radiation response by DNA ligands. University of Delhi.

8. Sharma, Rajan. 2001. Studies on hydroxamic acids and their thio analogues. University of Delhi.

7. Priyadarsiny, Priyanka. 2000. Investigations on a multifunctional allergen and antigen of *Aspergillus*

fumigates. University of Delhi.

6. Sarma, Bhupendra Kumar. 2000. Semiempirical SCFMO studies of the protomeric equilibria of alloxan. University of Delhi.

5. Katoch, Vandana. 1999. Theoretical studies on the protomeric equilibria of barbituric acid. University of Delhi.

4. Padhi, Bhabani S. 1997. Theoretical study of C_3H_4 and C_3H_3F isomers and their interconversions. University of Delhi.

3. Ramasami, P. 1997. Volume and compressibility studies of some amino carboxylic acids and a peptide in water and aqueous solutions of sodium sulphate at 288.15 K, 298.15 K and 308.15 K. University of Delhi.

2. Narula, Vinita. 1997. Volumetric and transport behaviour of some 1:1 electrolytes in ethanolamine and aqueous ethanolamine mixtures at 298.15 K. University of Delhi.

1. Walia, Vibha. 1992. Theoretical study of some unimolecular rearrangements. University of Delhi.

Supervision of Doctoral Thesis, under progress

Azad, Neeta. Computational study of PDHK inhibitors (15-02-2013).

Badhani, Bharti. Computational studies on antioxidants (15-02-2013).

Bansal, Perna. DFT studies on anti-ageing drugs (15-02-2013).

Arora, Ritu. Computational chemistry: Theoretical studies on amides (20-06-2013).

Radhika Rajesh

Supervision of awarded M.Phil dissertations

Azad, Neeta. 2010. AZ12 based design of PDHK inhibitors. University of Delhi.

Singh, Sarita. 2010. Metal ion selectivity of kojate complexes. University of Delhi.

Singh, Chayannika. 2009. Theoretical and spectral characterization of the kojic acid structure. University of Delhi.

Batra, Prinka. 2008. Structures and stabilities of small alkaline earth nanoparticle clusters. University of Delhi.

Tyagi, Prateek. 2008. Structural aspects of oxaliplatin: A combined theoretical and experimental study. University of Delhi.

Pathak, Mallika. 2003. A density functional study on the rearrangement of vinylidenes. University of Delhi.

Verma, Deepshikha. 2002. A theoretical study of the structure and unimolecular decomposition pathways of pyruvic acid. University of Delhi.

Pathy, Ajaya Kumar. 1993. The structure of the molecular and zwitterionic forms of anthranilic acid. University of Delhi.

Padhi, Bhabani Shankar. 1992. Theoretical study of the rearrangement of vinylidenes. University of Delhi.

Publications Profile

Book published

Rita Kakkar, *Atomic and Molecular Spectroscopy: Concepts and Applications*, Cambridge University Press: 2015. ISBN-13: 978-1107063884.

Research papers published in Refereed/Peer Reviewed Journals (last five years)

Bharti Badhani, Neha Sharma & **Rita Kakkar**. 2015. Gallic acid: a versatile antioxidant with promising therapeutic and industrial applications. *RSC Advances* **5**: 27540 – 27557.

Upasana Issar, Tripti Kumari & **Rita Kakkar**. 2015. Assessment of molecular binding of Hoechst 33258 analogues into DNA using docking and MM/GBSA approach. *Journal of Computational Science* 05/2015; DOI:10.1016/j.jocs.2015.05.003.

Neha Sharma & **Rita Kakkar**. 2015. Adsorption of sarin on MgO nanotubes: Role of doped and defect sites. *Journal of Computational Science* 01/2015; DOI:10.1016/j.jocs.2014.12.003.

Kumari, T., Upasana Issar & **Rita Kakkar**. 2014. Docking Modes of BB-3497 into the PDF Active Site – A Comparison of the Pure MM and QM/MM Based Docking Strategies. *Current Computer - Aided Drug Design* 12/2014; 10(4):315-26. DOI:10.2174/157340991004150518145522.

Kakkar, Rita; Arora, Richa; Gahlot, Pragya; Gupta, Deepti. 2014. An insight into pyruvate dehydrogenase kinase (PDHK) inhibition through pharmacophore modeling and QSAR studies. *J. Comput. Sci.* **5**: 558–567.

Kakkar, Rita, Sharma, Smriti; Badhani, Bharti. 2014. Density functional study of functionalization of carbon nanotubes with carbenes. *Can. Chem. Trans.* **2(4)**: 434-449.

Kohli, Esha; Arora, Ritu; **Kakkar, Rita**. 2014. Theoretical study of the stability of tautomers and conformers of isatin-3-thiosemicarbazone (IBT). *Can. Chem. Trans.* **2(3)**: 327-342.

Bansal, P.; **Kakkar, Rita**. 2014. Resveratrol: a polyphenol with multiple health benefits. *IJPDA*. 2(3): 174-191.

Khan, Rais Ahmad; Asim, Ahmad; **Kakkar, Rita**; Gupta, Deepti; Bagchi, Vivek; Arjmand, Farukh; Tabassum, Sartaj. 2013. A chloro-bridged heterobimetallic (η^6 -Arene) ruthenium–organotin complex as

an efficient topoisomerase α inhibitor. *Organometallics*. **32(9)**: 2546-2551.

Tyagi, Jyoti; **Kakkar, Rita** 2013 Surface affinity of graphene for health, energy and environmental safety applications. *Adv. Mat. Lett.* **4(10)**: 721-736.

Kakkar, R.; Bhandari, M., Gaba, R. 2013. DFT study of some trivalent d- and f-block metal ion complexes of alloxan. *J. Theor. Comput. Chem.* **12(6)**: 1350052 (18 pages)

Ramasami, Ponnadurai; Abdallah, Hassan H; Archibong, Edet F; Blowers, Paul; Ford, Thomas A; **Kakkar, Rita**; Shuai, Zhigang; Schaefer III, Henry F. 2013. Assessment of theoretical methods for the study of hydrogen abstraction kinetics of global warming gas species during their degradation and byproduct formation (IUPAC Technical Report) *Pure Appl. Chem.* **85(9)**: 1901-1918. DOI:<http://dx.doi.org/10.1351/PAC-REP-10-02-38>.

Batra, Prinka; Gaba, Ritu; Issar, Upasana; **Kakkar, Rita**. 2013. Structures and stabilities of alkaline earth metal oxide nanoclusters: A DFT study. *J. Theor. Chem.* **2013**, Article ID 720794, 14 pages. DOI:10.1155/2013/720794.

Gaba Ritu, Mamta Bhandari & **Rita Kakkar**. 2013. Adsorption studies of acetaldehyde on TiO₂ nanosurface. *Adv. Mater. Lett.* **4(10)**: 769-778 | DOI: 10.5185/amlett.2013.2424. doi. 10.5185/amlett.2013.2424.

Kakkar, Rita & Mamta Bhandari. 2013. Theoretical investigation of the alloxan-dialuric acid redox cycle. *Int. J. Quant. Chem.* **113(17)**: 2060-2069. DOI: 10.1002/qua.24441.

Gulia, Sunita & **Kakkar, Rita**. 2013. ZnO quantum dots for biomedical applications. *Adv. Mater. Lett.* **4(12)**, 876-887. DOI: 10.5185/amlett.2013.3440.

Malik, Pragati; Gulia, Sunita; **Kakkar, Rita**. 2013. Quantum dots for diagnosis of cancers. *Adv. Mater. Lett.* **4(11)**: 811-822 | DOI: 10.5185/amlett.2013.3437.

Singh, Sarita; Singh, Jyoti; Gulia, Sunita; **Kakkar, Rita**. 2013. Metal ion selectivity of kojate complexes: A theoretical study. *J. Theor. Chem.* Article ID 342783, 9 pages.

Upasana Issar & **Rita Kakkar**. 2013. DNA minor groove binder Hoechst 33258 and its analogues: a review. *Int. Rev. Biophys. Chem. (IREBIC)* 01/2013; **4(1)**: 49-66.

Tripti Kumari, Richa Arora & **Rita Kakkar**. 2013. Peptide Deformylase inhibitors for addressing the issue of bacterial resistance. *Int. Rev. Biophys. Chem. (IREBIC)* 01/2013; **4(1)**: 19-48.

Sharma, Neha & **Rita Kakkar**. 2013. Recent advancements on warfare agents/metal oxides surface chemistry and their simulants studies. *Adv. Mater. Lett.* **4(7)**: 508-521. doi. 10.5185/amlett.2012.12493.

Arora, Richa & **Rita Kakkar**. 2012. Benzohydroxamic acid and its applications. *Int. Rev. Biophys. Chem.* 3:

Kakkar, Rita, Neeta Azad & Pragya Gahlot. 2012. AZ12 based design of PDK2 inhibitors. *Int. Rev. Biophys.*

Chem. 3:

Kakkar, Rita, Mamta Bhandari & Ritu Gaba. 2012. Tautomeric transformations and reactivity of alloxan, *Comput. Theor. Chem.* 986: 14-24.

Kakkar, Rita. 2011. Structure-based design of PDHK2 inhibitors from docking studies. *Int. Res. J. Pharm.* 01: 02: 51-59.

Kakkar, Rita & Smriti Sharma. 2011. DFT Study of interactions of carbenes with boron nitride nanotubes. *J. Chem.* 01(01): 9-20.

Gahlot, Pragya and **Rita Kakkar**, 2011. Docking Modes of Pfz3 and its analogues into the lipoamide binding site on PDHK2. *Int. Res. J. Pharm.* 01 (01): 1-8.

Kakkar, Rita & Chayannika Singh. 2011. Theoretical study of the kojic acid structure in gas phase and aqueous solution. *Inter. J. Quant. Chem.* 111: n/a. doi: 10.1002/qua.22968.

Ojha, Himanshu, Pragya Gahlot, Anjani K. Tiwari, Mallika Pathak & **Rita Kakkar**. 2010. Quantitative structure activity relationship study of 2,4,6-trisubstituted-s-triazine derivatives as antimalarial inhibitors of *Plasmodium Falciparum* dihydrofolate reductase. *Chem. Biol. Drug Des.* 77: 57-62.

Sharma, S. N., U. Kumar, V. N. Singh, B. R. Mehta & **Rita Kakkar**, R. 2010. Surface modification of CdSe quantum dots for biosensing applications: Role of ligands. *Thin Solid Films* 519 (3): 1202-1212.

Gupta, Shweta, Nahar Singh, Murali Sastry, **Rita Kakkar** & Renu Pasricha. 2010. Controlling the assembly of hydrophobized gold nanoparticles at the air–water interface by varying the interfacial tension. *Thin Solid Films*. 519(3): 1072-1077.

Kumar, Umesh, Kusum Kumari, Shailesh N. Sharma, Mahesh Kumar, V. D. Vankar, **Rita Kakkar** and Vikram Kumar. 2010. Role of surface modification of colloidal CdSe quantum dots on the properties of hybrid organic–inorganic nanocomposites. *Colloid Polym. Sci.* 288(8): 841-849.

Sharma, Shailesh N., Umesh Kumar, T. Vats, M. Arora, V. Singh, B. R. Mehta, K. Jain, **Rita Kakkar** and A. K. Narula. 2010. Hybrid organic-inorganic (MEH-PPV/P3HT: CdSe) nanocomposites: Linking film morphology to photostability. *Eur. Phys. J. Appl. Phys.* 50(2): 206021-206027.

Kumar, Umesh, Shailesh N. Sharma, Sukhvir Singh, M. Kar, V.N. Singh, B.R. Mehta and **Rita Kakkar**. 2009. Size- and shape-controlled synthesis and properties of colloidal PbSe nanocrystals. *Mater. Chem. Phys.* 113(1): 107-114.

Kumari, Kusum, Umesh Kumar, Shailesh N Sharma, Suresh Chand, **Rita Kakkar**, V.D. Vankar and Vikram Kumar. 2008. Effect of surface passivating ligand on structural and optoelectronic properties of polymer: CdSe quantum dot composites. *J. Phys. D: Appl. Phys.* 41(23): 235409.

Tyagi, Prateek, Pragya Gahlot and **Rita Kakkar**. 2008. Structural aspects of the anti-cancer drug oxaliplatin: A combined theoretical and experimental study. *Polyhedron*. 27(18): 3567-3574.

Kakkar, Rita, Sheza Zaidi and Rajni Grover. 2008. The Curtius rearrangement of some organic azides: A DFT mechanistic study. *Inter. J. Quantum Chem.* 109(5): 1058-1069.

Sharma, Himani, Shailesh Sharma, Umesh Kumar, V Singh, B Mehta, Gurmeet Singh, S Shivaprasad and **Rita Kakkar**. 2008. Formation of water-soluble and biocompatible TOPO-capped CdSe quantum dots with efficient photoluminescence. *J. Mater. Sci.: Mater. Med.* 20 (Suppl. 1): 123-130. DOI: 10.1007/s10856-008-3494-2.

Kakkar, Rita, Mallika Pathak and Pragya Gahlot. 2008. Effect of aqueous solvation on the structures of pyruvic acid isomers and their reactions in solution: A computational study. *J. Phys. Org. Chem.* 21(1):23-29.

Kakkar, Rita, Amita Dua and Sheza Zaidi. 2007. Preparation, properties and infrared spectral studies of *N*-(*p*-ethylphenyl)thiobenzohydroxamic acid. *Spectrochimica Acta: A.* 68(5):1362-1369.

Kakkar, Rita, Amita Dua and Pragya Gahlot. 2007. Metal ion complexes of thioformin: A density functional study. *Polyhedron.* 26(18): 5301-5308.

Kakkar, Rita, Amita Dua and Sheza Zaidi. 2007. Density functional study of the conformations and intramolecular proton transfer in thiohydroxamic acids. *Org. Biomol. Chem.* 5(3):547-557. DOI: 10.1039/b610899g.

Research papers Published in Conferences/Seminar other than Refereed/Peer Reviewed Conferences

Sharma, S N, U Kumar, K Kumari, V D Vankar, **Rita Kakkar** and V Kumar. 2007. A novel non-TOPO route for the synthesis of colloidal CdSe quantum dots with high luminescence and stability. In proceedings *14th International Workshop on the Physics of Semiconductor Devices, IWPSD 2007*, December, 2007, Mumbai. Article number 4472652, 843-846.

Conference Organization/ Presentations (in the last three years)

Conference Organization

Organizing convener: Workshop on "Electronic Structure, atomistic and statistical modeling in chemistry, materials and life sciences", University of Delhi, October 8-10, 2014.

Conference Presentations

Smriti Sharma and **Rita Kakkar**. Density Functional study of functionalization of carbon nanotubes with carbenes. National Seminar on Current Trends in Chemistry- CrTriC 2011, Cochin University of Science and Technology, Oral Presentation, 4-5 March, 2011.

Azad, Neeta, Pragya Gahlot, Deepti Gupta and **Rita Kakkar**. AZ12 based Drug Designing of PDHK2 Inhibitors. Workshop on "Molecular Modelling & Drug Design", CMSD, University of Hyderabad, August 2-7, 2010. Poster presentation: 3rd prize.

Kumar, Umesh, Kusum Kumari, Shailesh N. Sharma, V.N. Singh, B.R. Mehta, V.D. Vankar, Vikram Kumar and **Rita Kakkar**. 2009. Hybrid Organic-Inorganic Nanocomposites: Linking Film Morphology to Photostability. Paper presented at the 18th International Photovoltaic Science and Engineering Conference and Exhibition, 19-22 January 2009, Kolkata, India.

Kumar, Umesh, Shailesh N Sharma, Kusum Kumari, **Rita Kakkar**, Vidyanand, B R Mehta, V D Vankar and Vikram Kumar. 2008. Role of ligands on the photophysics and photochemistry of colloidal CdSe quantum dots. Paper presented at the Asia Pacific Academy of Materials (APAM). 18-20 November, 2008, National Physical Laboratory, New Delhi, India.

Hassan H.Abdallah, Edet F. Archibong, Paul Blowers, Tony Ford, **Rita Kakkar**, Zhigang Shuai, Henry F. Schaefer III and Ponnadurai Ramasami. 2008. Theoretical Methods for the Study of Reactions Involving Global Warming Gas Species Degradation and Byproduct Formation. Paper presented at the *World Association of Theoretical and Computational Chemists Congress (WATOC 2008)*, September 15, 2008, Sydney, Australia.

Kumar, Umesh, S. N. Sharma, Mahesh Kumar, V. N. Singh, B.R. Mehta, **Rita Kakkar** and S. M. Shivaprasad. 2008. Role of different ligand in controlling the crystal size and size-distribution of colloidal CdSe nanocrystals. Paper presented at the 2nd International Conference on Advanced Nanomaterials, Aveiro, Portugal, June 2008.

Kumari, Kusum, Umesh Kumar, Shailesh N Sharma, V D Vankar, **Rita Kakkar** and Vikram Kumar. Hybrid organic-inorganic nanocomposites: Size dependence and stability studies. ABS11040ICAM. Paper presented at the *International Conference on Advanced Materials (ICAM-2008)*, February 18-21, 2008, Kottayam.

Sharma, S. N., Umesh Kumar, V. N. Singh, B. R. Mehta and **Rita Kakkar**. 2008. Toward greener nanosynthesis of core-shell CdSe-ZnSe quantum dots. International Conference on Nanomaterial Nanotoxicology (ICONTOX 2008), Feb. 2008, Lucknow.

Kumar, Umesh, KusumKumari, Shailesh N Sharma, V D Vankar, **Rita Kakkar** and Vikram Kumar. 2007. Effect of ligands on the properties of hybrid organic-inorganic nanocomposites. Paper presented at the *Indo-Australian symposium on multifunctional nanomaterials, nanostructures and applications (MNNA 2007)*, December 19-21, 2007, Department of Physics & Astrophysics, University of Delhi, Delhi.

Kumar, Umesh, Kusum Kumari, Shailesh N Sharma, V D Vankar, **Rita Kakkar** and Vikram Kumar. 2007. A novel non-TOPO route for the synthesis of colloidal CdSe quantum dots with high luminescence and stability. Paper presented at the 14th *International workshop on the physics of semiconductor devices (IWPSD-2007)*, December 16-20, 2007, Indian Institute of Technology, Bombay & Tata Institute of Fundamental Research (TIFR), Bombay.

Singh, Sukhvir, Umesh Kumar, Shailesh N. Sharma, N. C. Mehra and **Rita Kakkar**. Structural and morphological aspects of PbSe quantum Dots, National conference on Electron Microscopy & AlliedFields and XXIX Annual Meeting of EMSI, Nov., 26-28, 2007, New Delhi.

Kumar, Umesh, Shailesh N. Sharma, M. Kar, V. N. Singh, B. R. Mehta and **Rita Kakkar**. Role of ligands on the photophysics and photochemistry of colloidal CdSe quantum dots", presented at the 8th Workshop on Biosensors and Bioanalytical μ -techniques in environmental and clinical analysis, held at Goa, Oct. 3-6, 2007.

Grover, Rajni, Amita Dua, Pragya Gahlot, Sheza Zaidi, Smriti Sharma, Ritu Gaba, Mamta Bhandari, Prinka Batra, Deepti Gupta and **Rita Kakkar**. 2007. Studies on the conformations and metal ion selectivity of

hydroxamates and thiohydroxamates. Paper presented at the 9th CRSI National Symposium in Chemistry, February 1-4, 2007, Department of Chemistry, University of Delhi.

Invited Lectures

Research Projects (Major Grants/Research Collaboration)

Name of Project: Destructive decomposition of chemical warfare agents by nanocrystalline metal oxides: Theoretical and experimental studies.

Position in Project: Principal Investigator.

Period: 01/06/2012-31/05/2015

Funding Agency: CSIR, New Delhi

Grant: INR 19,92,000/-

Name of Project: Assessment of theoretical methods for the study of reactions involving global warming gas species degradation and by-product formation.

Position in Project: Member, Task Force.

Period: 12 December, 2007–December, 2009

Funding Agency: IUPAC Project

Grant: \$6000

Delhi University's Scheme to Strengthen Doctoral Research (April 2010-) >23 lakhs

7 Awards and Distinctions

Fellowship of Royal Society of Chemistry (London)

Association With Professional Bodies

Reviewing

Reviewer, Chemical Communications, Chemical Physics Letters, Dalton Transactions, Energy & Environmental Science, RSC, IEJMD, Journal of Luminescence, Elsevier, Journal of Molecular Modeling, Journal of Organic Chemistry, Journal of Physical Chemistry B, Journal of Physical Organic Chemistry, Journal of Solution Chemistry, New Journal of Chemistry, Organic & Biomolecular Chemistry, Organic Letters, Physical Chemistry Chemical Physics, Soft Matter, Tetrahedron, Theoretical Chemistry Accounts, Thermochemica Acta, Journal of Pharmacognosy & Phytotherapy, RSC Advances.

Reviewer, Chemistry books for various well-known publishers like Macmillan, McGraw-Hill and Pearson.

Advisory

ICCS 2007: Advancing Science and Society through Computation, Beijing, China, May 27-30, 2007.

ICCS 2008: International Conference on Computational Science- 3rd Workshop on computational chemistry and its applications at Kraków, Poland, June 23-25, 2008.

ICCS 2009: International Conference on Computational Science- 4th Workshop on computational chemistry and its applications: Compute. Discover. Innovate. at Baton Rouge, Louisiana, U.S.A., May 25-

27, 2009.

ICCS 2010: Celebrating 10 years of Advancing Computational Thinking. Computational Science, University of Amsterdam, The Netherlands, May 31 - June 2, 2010.

ICPAC 2010: The International Conference on Pure and Applied Chemistry (ICPAC 2010) held on July 26-30, 2010, University of Mauritius, <http://www.uom.ac.mu/icpac/design/html/intcom.html>.

ICCS 2011: The Ascent of Computational Excellence. June 1 - June 3, 2011, Nanyang Technical University, Singapore.

ICCS 2012: Empowering Science through Computing. June 4 - June 6, 2012, Omaha, Nebraska.

ICCS 2013: Computation at the Frontiers of Science, Barcelona, Spain, June 5 - June 7, 2013.

ICCS 2014: Big Data meets Computational Science, Cairns, Australia, 10-12 June, 2014.

Committees and Boards

Member, University Grants Commission, CBCS Syllabus Committee.

Member, University Grants Commission Expert and Advisory Committees of various Universities.

Member, Syllabus Revision Committees of Dyal Bagh University, Agra, 2010, 2015.

Memberships

Fellow, Royal Society of Chemistry (London)

American Chemical Society (ACS)

Life Member, Chemical Research Society of India (CRSI).

Member, Asian Council of Science Editors

Editorial Boards

American Journal of Quantitative Spectroscopy

Other Activities

Book:

Rita Kakkar, Atomic & Molecular Spectroscopy: Basic Concepts & Applications, Cambridge University Press.

Chapter in Book:

Kakkar, R. Theoretical studies on hydroxamic acids. 2013. Chapter in book *Hydroxamic Acids*. Ed. S. P. Gupta. Springer Berlin-Hiedelberg, 19-53. ISBN: 978-3-642-38110-2 (print); 978-3-642-38111-9 (e-book).