




Faculty Details proforma for DU Web-site

Title	Prof.	First Name	Rita	Last Name	Kakkar	Photograph
Designation	Professor					
Address	Off. Department of Chemistry, University of Delhi, Delhi-110007.					
Phone No Office	01127666646 Ext. 204					
Residence	01127666313					
Mobile	9810120508					
Email	ritakakkar10@gmail.com, rita@kakkar@co.in, 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						
1981 – 1984 Lecturer, Miranda House, University of Delhi. 1984 onwards: Department of Chemistry, University of Delhi (presently Professor).						
Administrative Assignments						
<p>Member, UGC Syllabus Committee for Choice Based Credit System. Ex-Member, Board of Studies, Dyal Bagh Institute, Agra Member, Board of Studies, Central University of Haryana, Mahendergarh. Coordinator, B. Sc. Chemistry Examinations (2010-2012), (2014-2017) Provost, Undergraduate Hostel for Girls (UGHG), Delhi University (2014 onwards) Provost, North Eastern Students' House for Women (NESHW), Delhi University (2007-2010). Former 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 & 2019-). Convener, Library Committee, Department of Chemistry, University of Delhi (2014-2017). Member (Board of Research Studies in Science, 2016-2017. Chairperson, Bhaskaracharya College of Applied Sciences, University of Delhi. Chairperson, WUS Working Women's Hostel, University of Delhi</p>						
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**

45. Ms. Kriti Kashyap. Achieving selective inhibition of Histone Deacetylase isoforms: an *in silico* approach. (Thesis submitted, 2019) University of Delhi.

44. Ms. Anshika Mittal. *In silico* studies of enzymes and their inhibitors. (Thesis submitted, 2019), University of Delhi.

43. Mandeep. 2019. DFT study of catalysis on nanosurfaces. University of Delhi.

42. Lekha Sharma. 2018. Hierarchically structured magnesium based oxides: Synthesis and applications in pesticide remediation. University of Delhi.

41. Ritu Arora. 2018. DFT Mechanistic studies on some rearrangement reactions, University of Delhi.

40. Radhika N.P. 2018. Synthesis, characterization and catalytic applications of hierarchical and nano zeolites for Friedel-Crafts alkylations. University of Delhi.

39. Arora, Ritu. 2017. DFT mechanistic studies on some important organic rearrangements. University of Delhi.

38. Badhani, Bharti. 2016. Investigation of varied facets of gallic acid: An *in silico* approach. University of Delhi.

37. Azad, Neeta. 2016. Novel pyruvate dehydrogenase kinase (PDHK) inhibitors based on *in silico* studies. University of Delhi.

36. Bansal, Perna. 2016. DFT studies of trans-resveratrol as an antioxidant and anti-ageing drug for activating sirtuins. University of Delhi.

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

34. Arora, Richa. 2014. *In silico* studies of hydroxamic acids and their biological applications. University of Delhi.
33. Malik, Pragati. 2014. Theoretical studies on some quantum dots. University of Delhi.
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). University of Delhi.
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.
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

Mr. Jogender, DFT study of adsorption of gases on graphene system.

Ms. Sonam, *In silico* studies of 4-thiazolidinones acting on E. Coli MurB protein.

Ms. Mudita Nagpal, Metal oxide assisted removal of chemical warfare agents.

Mr. Ankit Mittal

Ms. Archa Gulati

Mr. Varun

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.

Chapters in books

6. Archa Gulati & Rita Kakkar (2018) DFT studies on storage and adsorption capacities of gases on MOFs: Advances in Applications.

5. Sonam Nirwan & Rita Kakkar (2019) Rhinovirus RNA Polymerase.

4. Kriti Kashyap & Rita Kakkar. 2017. Herpesvirus Proteases & Their Inhibitors. Chapter in book: Viral Proteases & Their Inhibitors. Ed. Satya P. Gupta. Academic Press. ISBN: 978-0-12-809712-0 (Print), 978-0-12-809682-6 (e-book).

3. Rita Kakkar. 2017. In Silico Design of PDHK Inhibitors: From Small Molecules to Large Fluorinated Compounds. Chapter in book: Computational Chemistry Methodology in Structural Biology and Materials Sciences. Eds. Tanmoy Chakraborty, Prabhat Ranjan, Anand Pandey. Apple Academic Press (CRC Press) Taylor & Francis. ISBN: 9781771885683.

2. Rita Kakkar & Mamta Bhandari. 2017. Pyruvate Dehydrogenase Kinases (PDHKs) and their Inhibition: A Possible Line of Treatment for Diabetes, Heart Ischemia and Cancer. Chapter in book: Advances in Studies on Enzyme Inhibition, Vol. 2: Miscellaneous Drugs. Ed. S. P. Gupta. Nova Science Publishers: New York. pp. 91-112. ISBN: 2474-9524 (Print); 978-1-53610-521-6 (e-book).

1. Rita Kakkar. 2013. Theoretical Studies on Hydroxamic Acids. Chapter in Book Hydroxamic Acids. A Unique Family of Chemicals with Multiple Biological Activities. Ed. S. P. Gupta. Springer-Heidelberg. pp. 19-53. ISBN: 978-3-642-38110-2 (Print); 978-3-642-38111-9 (Online).

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

151. Sonam Nirwan, Varun Chahal & Rita Kakkar (2020) Theoretical study of the structural features and antioxidant potential of 4-thiazolidinones. *Struct. Chem.* 23 March 2020. IF: 1.624.

150. Mudita Nagpal & Rita Kakkar (2020) Facile synthesis of mesoporous magnesium oxide–graphene oxide composite for efficient and highly selective adsorption of hazardous anionic dyes. *Res. Chem. Intermediates*. DOI: 10.1007/s11164-020-04103-0. IF: 2.064.

149. Sonam Nirwan, Varun Chahal & Rita Kakkar (2020) Structure-based virtual screening, free energy of binding and molecular dynamics simulations to propose novel inhibitors of Mtb-MurB oxidoreductase enzyme. *J. Biomol. Struct. Dyn.* 2020 Jan 25:1-16. doi: 10.1080/07391102.2020.1712258. IF: 3.310.

148. Mudita Nagpal & Rita Kakkar (2020) Adsorptive Degradation of Phosmet Using Hierarchically Porous Calcium Oxide: An Experimental and Theoretical Study. *ChemistrySelect*. 5: 1235-1246. IF: 1.716.

147. Kriti Kashyap & Rita Kakkar (2020) Exploring structural requirements of isoform selective histone deacetylase inhibitors: a comparative in silico study. *J. Biomol. Struct. Dyn.* DOI: <https://doi.org/10.1080/07391102.2019.1711191>. IF: 3.310.

146. Mandeep, Archa Gulati & Rita Kakkar (2020) DFT study of adsorption of glyphosate pesticide on Pt-Cu decorated pyridine-like nitrogen-doped graphene. *J. Nanoparticle Res.* **Volume 22**, Article number: 17 (2020). IF: 2.009.
145. Mandeep, Archa Gulati & Rita Kakkar (2019) Graphene-based adsorbents for water remediation by removal of organic pollutants: Theoretical and experimental insights. *Chem. Engg. Res. Des.* DOI: [10.1016/j.cherd.2019.10.013](https://doi.org/10.1016/j.cherd.2019.10.013) IF: 3.073.
144. Varun Chahal, Sonam Nirwan & Rita Kakkar (2019) Combined approach of homology modeling, molecular dynamics, and docking: computer-aided drug discovery. *Phys. Sci. Rev.* **4(10)** DOI: [10.1515/psr-2019-0066](https://doi.org/10.1515/psr-2019-0066).
143. Zhi Tan, Lekha Sharma, Rita Kakkar, [...], Minhua Cao (2019) Arousing the Reactive Fe Sites in Pyrite (FeS₂) via Integration of Electronic Structure Reconfiguration and in Situ Electrochemical Topotactic Transformation for Highly Efficient Oxygen Evolution Reaction. *Inorg. Chem.* **58 (11)** 7615-7627. IF: 4.850.
142. Mandeep, Lekha Sharma & Rita Kakkar (2019) Adsorption of Bromonitromethane over Graphene-Based Substrates: A Density Functional Theory Analysis. *ChemistrySelect.* **4(17)**: 4967-4974. IF: 1.716.
141. Ritu Arora, Kriti Kashyap, Anshika Mittal & Rita Kakkar (2019) Synthesis and Reactions of Diazoketones. *Org. Prep. Proced. Int.* **51(2)**: 103-146. IF: 1.520.
140. Anu Sharma, Anita Yadav, Nikesh Gupta, Sandeep Sharma, Rita Kakkar, [...], Rakesh Kumar Sharma (2019) Multifunctional mesoporous Curcumin Encapsulated Iron-Phenanthroline Nanocluster: A New Anti-HIV agent. *Colloids and Surfaces B: Biointerfaces.* **180**: 289-297. IF: 2.997.
139. Sonam Nirwan, Varun Chahal & Rita Kakkar (2019) Thiazolidinones: Synthesis, Reactivity, and Their Biological Applications. *J. Heterocycl. Chem.* **56(4)**: 1239-1253. IF: 1.241.
138. Anshika Mittal & Rita Kakkar (2019) Nitric Oxide Synthases and Their Inhibitors: A Review. *Lett. Drug Des. Discovery.* DOI: [10.2174/1570180816666190222154457](https://doi.org/10.2174/1570180816666190222154457).
137. Varun Chahal, Sonam Nirwan & Rita Kakkar (2019) Isatin and its derivatives: A survey of recent syntheses, reactions, and applications. *Med. Chem. Commun.* **10**: 351-368. IF: 2.495.
136. Kriti Kashyap & Rita Kakkar (2019) An insight into selective and potent inhibition of Histone Deacetylase 8 through induced-fit docking, pharmacophore modeling and QSAR studies. *J. Biomol. Struct. Dyn.* **38(1)**: 48-65. IF: 3.310.
135. Upasana Issar, Richa Arora, Tripti Kumari & Rita Kakkar (2019) Combined pharmacophore-guided 3D-QSAR, molecular docking, and virtual screening on bis-benzimidazoles and ter-benzimidazoles as DNA-topoisomerase I poisons. *Struct. Chem.* **30**: 1185-1201. IF: 1.624.
134. Anshika Mittal, Ritu Arora & Rita Kakkar (2018) Pharmacophore Modeling, 3D-QSAR and Molecular Docking Studies of Quinazolines and Aminopyridines as Selective Inhibitors of Inducible Nitric Oxide

Synthase. *J. Theor. Comput. Chem.* **18(1)** 1950002.

133. Richa Arora, Upasana Issar & Rita Kakkar (2018) Identification of novel urease inhibitors: pharmacophore modeling, virtual screening and molecular docking studies. *J. Biomol. Struct. Dyn.* **37(16)**: 4312-4326. IF: 3.310.

132. N.P. Radhika, Rosilda Selvin, Rita Kakkar, [...], Hsui Ling Hsiu (2018) Tertiary Butylation of Aniline Over Nanosized Zeolite Beta Catalyst. *J. Nanosci. Nanotech.* **18**: 7960-7968. IF: 1.354.

131. Lekha Sharma & Rita Kakkar (2018) Magnetically retrievable one-pot fabrication of mesoporous magnesium ferrite (MgFe₂O₄) for the remediation of chlorpyrifos and real pesticide wastewater. *J. Environ. Chem. Engg.* **6(6)**: 6891-6903. IF: 4.020.

130. Mudita Nagpal & Rita Kakkar (2018) Use of metal oxides for the adsorptive removal of toxic organic pollutants. *Separation & Purification Technology*. DOI: [10.1016/j.seppur.2018.10.016](https://doi.org/10.1016/j.seppur.2018.10.016). IF: 5.107.

129. Navneet Sharma, Rita Kakkar, Prerna Bansal, [...], Rakesh Kumar (2019) Host-guest complexation studies of p-tertbutylcalix[4]arene against ions of interest for radiological decontamination. *Inorg. Chim. Acta.* **484(1)**: 111-124. IF: 2.046.

128. Richa Arora, Upasana Issar & Rita Kakkar (2018) Theoretical investigation of organotin(IV) complexes of substituted benzohydroxamic acids. *Comput. Theor. Chem.* **1138**: 57-65. IF: 1.344.

127. Mandeep, Lekha Sharma & Rita Kakkar (2018) DFT study on the adsorption of p-nitrophenol over vacancy and Pt-doped graphene sheets. *Comput. Theor. Chem.* **1142(15)**: 88-96. IF: 1.344.

126. N.P. Radhika, Rosilda Selvin, Rita Kakkar & L. Selva Roselin (2018) Nanocrystalline Hierarchical ZSM-5: An Efficient Catalyst for the Alkylation of Phenol with Cyclohexene. *J. Nanosci. Nanotech.* **18(8)**: 5404-5413. IF: 1.354.

125. Archa Gulati & Rita Kakkar (2018) DFT studies on storage and adsorption capacities of gases on MOFs. *Phys. Sci. Rev.* **3(8)**. DOI: <https://doi.org/10.1515/psr-2017-0196>.

124. Ruchi Jain, Parveen Gahlyan, Sonam Dwivedi, [...], Mamta Bhandari, Ritu Arora, Rita Kakkar, Ashok Prasad (2018) Design, Synthesis and Evaluation of 1 H -1,2,3-Triazol-4-yl-methyl Tethered 3-Pyrrolylisatins as Potent Anti-Breast Cancer Agents. *ChemistrySelect.* **3(19)**: 5263-5268. IF: 1.716.

123. Mudita Nagpal & Rita Kakkar (2018) An evolving energy solution: Intermediate hydrogen storage. *Int. J. Hydrogen Energy.* **43(27)**: 12168-12188. IF: 4.229.

122. Ritu Arora, Kriti Kashyap & Rita Kakkar (2018) Rearrangements in Radical Cations of Diazoketones: A DFT Mechanistic Study. *Comput. Theor. Chem.* **51(2)**: 103-146. IF: 1.344.

121. Bharti Badhani & Rita Kakkar (2017) Influence of intrinsic and extrinsic factors on the antiradical activity of Gallic acid: a theoretical study, *Struct. Chem.* **29**: 359-373. IF: 1.624.

120. Richa Arora, Upasana Issar & Rita Kakkar (2018) In silico study of the active site of Helicobacter

- pylori urease and its inhibition by hydroxamic acids. *J. Mol. Graph. Model.* **183**: 64-73. IF: 1.863.
119. Pragati Mallik & **Rita Kakkar** (2018) Effects of increasing number of rings on the ion sensing ability of CdSe quantum dots: a theoretical study. *J. Nanopart. Res.* Apr. **20**. Article number 114. IF: 2.009.
118. Mallika Pathak, Himanshu Ojha, ...& **Rita Kakkar**, Design, synthesis and biological evaluation of antimalarial activity of new derivatives of 2,4,6-s-triazine. *Chem. Central J.* 11 (1) 132 **2017**. DOI 10.1186/s13065-017-0362-5. Impact Factor: 1.027.
117. Lekha Sharma & **Rita Kakkar**, Hierarchically structured Magnesium based oxides: Synthesis strategies and applications in organic pollutant remediation. *CrystEngComm* 19(46) 6913-6926. **2017**. DOI: 10.1039/C7CE01755C. Impact Factor: 3.474.
116. Badhani, B. & **Rita Kakkar**, Structural, electronic, and reactivity parameters of some triorganotin(IV) carboxylates: a DFT analysis, *Struct. Chem.* 1-11 **2017**. DOI 10.1007/s11224-017-1068-y. Impact Factor: 1.854.
115. Lekha Sharma & **Rita Kakkar**, Hierarchical Porous Magnesium Oxide (Hr-MgO) Microspheres for Adsorption of an Organophosphate Pesticide: Kinetics, Isotherm, Thermodynamics, and DFT Studies, *ACS Appl. Mater. Interfaces*, **2017**. DOI: 10.1021/acsami.7b14370. Impact Factor: 7.504.
114. Rakesh Kumar, Parveen Gahlyan, Neha Yadav, Mamta Bhandari, **Rita Kakkar**, Manu Dalela & Ashok K. Prasad, Bis -triazolylated-1,4-dihydropyridine - Highly selective hydrophilic fluorescent probe for detection of Fe³⁺. **2017**. *Dyes and Pigments* 147: 420-428. DOI: 10.1016/j.dyepig.2017.08.048. Impact Factor: 3.473.
113. Badhani, B. & **Kakkar, Rita** DFT study of structural and electronic properties of gallic acid and its anions in gas phase and in aqueous solution. *Struct. Chem.* **2017**. doi:10.1007/s11224-017-0958-3. Impact Factor: 1.854.
- 112. Kakkar, Rita**, Arora, R. & Zaidi, S. DFT studies on the acid-catalyzed Curtius reaction: the Schmidt reaction. *Struct. Chem.* **2017**, 28(6), 1743-1756. Impact Factor: 1.854.
111. Issar, U., Kumari, T., Arora, R. & **Kakkar, Rita** Conformational properties of DNA minor groove binder Hoechst 33258 in gas phase and in aqueous solution. *Comp. Theor. Chem.* **2017**, 1113, 32-41. Impact Factor: 1.403.
110. Kumar, R., Yadav, N., Lavilla, R., Blasi, D., Quintana, J., Brea, J. M., Loza, M.I., Mestres, J., Bhandari, M., Arora, R., **Kakkar, Rita** & Prasad, A. K. Synthesis, pharmacological evaluation and molecular docking of pyranopyrazole-linked 1,4-dihydropyridines as potent positive inotropes. *Mol. Divers.* **2017**. doi:10.1007/s11030-017-9738-7. Impact Factor: 1.896.
109. Arora, Ritu & **Kakkar, Rita** Negative Ion Wolff Rearrangement of Some Diazoketones: A Theoretical Mechanistic Study. *Comp. Theor. Chem.* **2017**, 1106, 50-57. Impact Factor: 1.403.
108. Arora, Richa, Issar, Upasana & **Kakkar, Rita**. Theoretical Study of the Molecular Structure and Intramolecular Proton Transfer in Benzohydroxamic Acid. *Comp. Theor. Chem.* **2017**, 1105, 18-26.

Impact Factor: 1.403.

107. Radhika, N.P; Selvin, R.; **Kakkar, Rita**; Hsu, H-L. Nanocrystals of Zeolite ZSM-5 as Catalysts for the Liquid Phase Benzoylation of Anisole with Benzyl Alcohol. *J. Nanosci. & Nanotech.* **2017**, *17(2)*, 1329-1337. Impact Factor: 1.338.

106. Arora, Ritu; **Kakkar, Rita**. Theoretical Study of the Mechanism of the Wolff Rearrangement of Some Diazocarbonyl Compounds. *Comp. Theor. Chem.* **2016**, *1094*, 32-41. Impact Factor: 1.403.

105. Radhika, N. P.; Selvin, R.; **Kakkar, Rita**; Umar, A. Recent Advances in Nano-photocatalysts for Organic Synthesis. *Arabian J. Chem.* **2016**, in press. Impact Factor: 3.613.

104. Badhani, Bharti; **Kakkar, Rita** *In silico* Studies on Potential MCF-7 Inhibitors: A Combination of Pharmacophore and 3D-QSAR Modeling, Virtual Screening, Molecular Docking, and Pharmacokinetic Analysis. *J. Biomol. Str. Dyn.* **2016**, *12*, 1-18. Impact Factor: 3.310.

103. Sharma, D.; Ojha, Himanshu; Pathak, Mallika; Singh, B.; Sharma, N.; Singh, A.; **Kakkar, Rita**; Sharma, R. K. Spectroscopic and Molecular Modeling Studies of Binding Mechanism of Metformin with Bovine Serum Albumin. *J. Mol. Struct.* **2016**, *1118*, 267-274. Impact Factor: 1.780.

102. Badhani, Bharti; Sharma, Neha; **Kakkar, Rita**. Gallic Acid: A versatile Antioxidant with Promising Therapeutic and Industrial Applications. *RSC Adv.* **2016**, *5*, 27540 – 27557. Impact Factor: 3.289.

101. Upasana Issar, Tripti Kumari & **Rita Kakkar**. Assessment of molecular binding of Hoechst 33258 analogues into DNA using docking and MM/GBSA approach. *J. Comput. Sci.* **2015**, *10*, 166-177. Impact Factor: 1.748.

100. Neha Sharma & **Rita Kakkar**. Adsorption of sarin on MgO nanotubes: Role of doped and defect sites. *J. Comput. Sci.* **2015**, *10*, 225-236. Impact Factor: 1.748.

99. Kumari, T., Upasana Issar & **Rita Kakkar**. 2014. Docking Modes of BB-3497 into the PDH Active Site – A Comparison of the Pure MM and QM/MM Based Docking Strategies. *Curr. Comput.-Aided Drug Des.* **2014**, *10(4)*, 315-326. Impact Factor: 1.151.

98. 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. Impact Factor: 1.748.

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

96. 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.

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

94. 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. Impact Factor: 3.862.
93. Tyagi, Jyoti; **Kakkar, Rita** 2013 Surface affinity of graphene for health, energy and environmental safety applications. *Adv. Mat. Lett.* **4(10)**: 721-736.
- 92. 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)
91. 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.
90. 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.
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Research papers Published in Conferences/Seminar other than Refereed/Peer Reviewed Conferences

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

Invited Lectures Several in various conferences, national and international.

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/-

Delhi University's Scheme to Strengthen Doctoral Research (April 2010-) >29 lakhs

7 Awards and Distinctions

Fellowship of Royal Society of Chemistry (London)
American Chemical Society

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, Journal of Hazardous Materials.

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 Dayal 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

Journal of Biochemistry and Molecular Biology Research (*ISSN 2313-7177*)

Other Activities

Signature of Faculty Member