

Pankaz K. Sharma, Ph.D.

Professor

Department of Chemistry

Cotton University

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Areas of Expertise

- Applied Theoretical/Computational Chemistry
- Computational Biophysics/Biochemistry
- Computational Bioinorganic Chemistry

Key Skills

- Advanced theoretical chemistry background
- Expertise in *ab-initio* MO and hybrid Density Functional Theory (DFT) calculations
- Extensive experience with computations of clusters and metalloenzyme active sites
- Authored or co-authored research papers and review articles for peer-reviewed, reputed journals
- Experienced with, and comfortable in, collaborative environment
- Proficiency in written and verbal English
- Strong communication skills
- Love and flair for teaching

Software Proficiency

Program Packages

Gaussian, Jaguar, GAMESS, Spartan, OCRA, Psi4

Visualization and Graphics Software

Adobe Illustrator, PiMol, VMD, ChemOffice, ChemCraft

Platforms

UNIX, Linux, and Windows

Academic Qualifications:

Ph.D. (Applied Theoretical Chemistry)

University of Hyderabad, India (2002)

Title of the Ph.D. Thesis

Theoretical Study on Cage and Bowl Shaped Molecules and Transition Metal-Group 14 Multiple Bonding

(Thesis submitted: June, 2001; Degree awarded: April, 2002).

Thesis Supervisor:

Prof. E. D. Jemmis, Former Director, IISER, Trivandrum

M.Sc. (Physical Chemistry)

University of Delhi, India (1995)

B.Sc. (Major: Chemistry)

Gauhati University, India (1991)

Employment History

Post-Ph.D. Teaching Experience:

1) Professor in Chemistry

Cotton University

Panbazar, Guwahati 781001 (June, 2023 – present)

2) Associate Professor in Chemistry

Cotton University

Panbazar, Guwahati 781001 (June, 2017 – June, 2023)

3) Associate Professor in Chemistry

Cotton College State University

Panbazar, Guwahati 781001 (**March, 2015 – June, 2017**)

4) Assistant Professor in Computational Sciences

Department of Chemistry, Sir Syed College (September, 2012 – December, 2012)

Sir Syed College, Karimbam 670 142, Taliparamba, Kannur (Dist) Kerala (INDIA)

Post-Ph.D. Research Experiences (12 years and 4 months)

1) Research Professor (Jan. 2013 – Oct, 2014) and Brain Pool Researcher (Apr. 2013 – March, 2013)

College of Pharmacy and School of Pharmaceutical Sciences, Ewha Womans University, Seoul

2) Research Associate (Nov. 2008 – Apr. 2012)

Department of Chemistry, University of Southern California (December, 2003-April, 2012)

Supervisor: Professor Arie Warshel, USC Distinguished Professor (**Nobel Prize in Chemistry, 2013**)

3) Postdoctoral Research Associate (Dec. 2003 – Nov. 2008)

Department of Chemistry, University of Southern California (December, 2003-April, 2012)

Supervisor: Professor Arie Warshel, USC Distinguished Professor (**Nobel Prize in Chemistry, 2013**)

4) Postdoctoral Fellow (Jun. 2001– Nov. 2003)

Department of Organic Chemistry, Hebrew University of Jerusalem, Israel

Supervisor: Professor Sason Shaik, Director of Lise Meitner Minerva Center for Computational Quantum Chemistry, Hebrew University of Jerusalem

Professional Experiences

Grant Applications for External Funding

• Assisted Professor Arie Warshel in writing several successful grant applications (**2005–2012**) to the National Institutes of Health (NIH), USA, and the National Science Foundation (NSF), USA

Total grant award amount: Several million US dollars.

• Independently written a successful grant application (on behalf of Ewha Womans University, Seoul) to the *Clare Boothe Luce Foundation* under their **Expanding Horizons** initiative (awarded in November, **2013**).

Grant award amount: USD 1.5 million (for a period of 3 years)

Administrative Duties Discharged:

1) Member, Academic Council, Cotton University (**2023** - till date)

2) Member, Executive Council, Cotton College State University (**2015 - 2017**)

3) Member, Academic Council, Cotton College State University (**2015 - 2017**)

4) Member, University Court, Cotton College State University (**2015 - 2017**)

5) Superintendent, KKH PG Boys' Hostel, Cotton College State University (July, **2015**- June, **2016**)

6) In charge, Students' Welfare, Cotton College State University (**2015- 2016**)

7) Assistant Chief Election Officer, Cotton College State University Students' Union Election, **2015** and **2016**.

Other Academic Duties Discharged:

1) Deputy Coordinator, Core Committee for the implementation of Modified and Upgraded CBCS Course in the Undergraduate and the Post-Graduate levels, Cotton University, **2017-2018**.

2) Deputy Convener, Post-Graduate Admission Committee, Cotton University, **2023**.

3) Deputy Convener, Post-Graduate Admission Entrance Examination, Cotton University, **2022**.

- 4) Member, Post-Graduate Admission Committee, Cotton University, **2015-2022**.
- 5) Observer, Post-Graduate Admission Entrance Examination, Cotton University, **2019**.
- 6) Adviser, Post-Graduate Admission Co-ordination Committee, Cotton University, **2024**.

External Academic Duties & Experiences

- 1) External Examiner for M.Sc. (Physical Chemistry) Project/Dissertation work, Manipur University (**2024**).
- 2) Subject Expert (Chemistry) for Recruitment of Common Education Services Examination 2023, Nagaland Public Service Commission (**2024**)
- 3) Selection committee member for recruitment of Project Scientific Officer at the Centre of Plasma Physics-Institute for Plasma Research (CPP-IPR), Sonapur, Kamrup (M), Assam (**2021**)
- 4) Expert member for the selection of JRF (for the Ph. D Programme 2015-16), at the Institute of Advanced Study in Science and Technology (IASST), Guwahati (**2015**)
- 5) **Ph.D. Thesis examiner:**
 - a) Gauhati University, Guwahati, Assam.
 - b) Panjab University, Chandigarh.
- 6) Reviewer for research journals of:
 - a) The American Chemical Society
 - b) The Royal Society of Chemistry, England
 - c) John Wiley & Sons, Inc.
 - d) The Elsevier Publishing Company
 - e) Springer (and Nature Springer)

Representative Duties Discharged:

- 1) General Secretary, Cotton College State University Teachers' Association (**2015-2017**)

Scientific Talks Organized

- 1) ***Boron Plays Hide and Seek: Inevitability of Uncertainties***, by Prof. E. D. Jemmis (Indian Institute of Science, Bangalore), at the Department of Chemistry, Cotton University, Guwahati (November, **2018**)
- 2) ***2, 6, 8, 20.... Just Count the Electrons. Electron Counting Rules and Structure and Stability of the Clusters***, by Prof. Kiran Boggavarapu (McNeese State University, LA, USA), at the Department of Chemistry, Cotton University, Guwahati (June, **2017**).

Supervisory Role:

Number of M.Sc. project students supervised: **10**

Number of Ph.D. students guided: **3** (one degree awarded; two pursuing)

Thesis Titles of the Ph.D. Students:

1. **Lakhya Jyoti Mazumder** - *Computational Studies of Non-Covalent Interactions in Super Tocopherol Derivatives and Nobel Gas Compounds* (PhD degree awarded in May, 2023).
2. **Rohan Sharma** - *In silico Studies of Noncovalent Interactions and Charge Transfer in Ring Systems, and Electronic Structure Analyses of Bowl-shaped Compounds* (Final Registration seminar presented)

3. **Farnaz Yashmin** - *Computational Studies of Interaction of Noble Gases with Neutral and Cationic Systems, Noble Gas Encapsulated Complexes and Electronic Structural Stability of Noble Gas Dimers* (Pre-Thesis Submission Seminar presented)

List of Peer-Reviewed Research Publications (Updated in July, 2025):

Total Citations: 5,490 (Google Scholar); 4,567 (Scopus); 4,238 (Web of Science); 4,990 (ResearchGate)

h-index: 25 (Google Scholar); 26 (Scopus); 24 (Web of Science); 26 (ResearchGate)

i10-index: 31 (Google Scholar)

1. *Computational Investigation of Cytochrome P450-Catalyzed Oxetane Formation in Taxol Biosynthesis*. Surajit Nandi, Rohan Sharma, Subhajit Mandal, Pankaz K. Sharma, Parayil Kumaran Ajikumar and Anakuthil Anoop, *Biochemistry*, **2025**, <https://doi.org/10.1021/acs.biochem.5c00175>
2. *Ng@M10H10: Nobel Gas Trapping by an Alkali Hydride Cage*. Farnaz Yashmin, Kangkan Sarmah, Pankaz K. Sharma and Ankur K. Guha, *Phys. Chem. Chem. Phys.* **2025** <https://doi.org/10.1039/D5CP01273B>
3. *Assessment of Charge Transfer Energies of Noncovalently Bounded Ar-TCNE Complexes Using Range-separated Density Functionals and Double Hybrid Density Functionals*. Rohan Sharma, Chayanika Kashyap, Trishna Kalita and Pankaz K. Sharma, *ChemPhysChem*, **2024** <https://doi.org/10.1002/cphc.202400784>.
4. *Computational Study of Noncovalent Interactions on Addition of Small Molecule Units with Benzenoid Aromatic Rings*. Rohan Sharma, Chayanika Kashyap, Drishti Baruah, Ilakshi Baruah and Pankaz K. Sharma, *Int. J. Quant. Chem.*, **2024**, 124, e27466 <https://doi.org/10.1002/qua.27466>
5. *Novel 2-mercaptobenzothiazole and 2-mercaptobenzimidazole Derived Novel Ag₁₆ and Ag₁₈ Nanoclusters: Synthesis and Optical Properties*. Bedanta Borah, Rohan Sharma, Pankaz K. Sharma and Apurba Kr. Barman, *Nanoscale*, **2024**, 16, 14844-14852 <https://doi.org/10.1039/D4NR01606H>
6. *Spodium Bonding with Noble Gas Atoms*. Farnaz Yashmin, Lakhya J. Mazumder, Pankaz K. Sharma and Ankur K. Guha, *Physical Chemistry Chemical Physics*, **2024** 26, 8115-8124 <https://doi.org/10.1039/D3CP06184A>
7. *Noble Gas Dative Bonding with Coinage Metal Carbene Complexes: A Theoretical Study*. Farnaz Yashmin, Rohan Sharma, Lakhya J. Mazumder and Pankaz K. Sharma, *J. Comput. Chem.* **2023**, 45, 536-545 <https://doi.org/10.1002/jcc.27253>
8. *Coordination of Noble Gases by Alkali-metal-like Superatom Cation Be₃B⁺*. Farnaz Yashmin, Lakhya J. Mazumder, Rohan Sharma and Pankaz K. Sharma, *J. Comp. Chem.*, **2023**, 44, 1733-1739. <https://doi.org/10.1002/jcc.27122>
9. *Beryllium Bonding With Noble Gas Atoms*. Lakhya Jyoti Mazumder, Rohan Sharma, Farnaz Yashmin and Pankaz Kumar Sharma, *J. Comp. Chem.*, **2023**, 44, 644-655. <https://doi.org/10.1002/jcc.27028>
10. *In-silico Exploration of Noble Gas Dimer Enforced by Noncovalent Interaction*. Lakhya J. Mazumder, Farnaz Yashmin and Pankaz K. Sharma, *Int. J. Quant. Chem.*, **2023**, 123, e27018, <https://doi.org/10.1002/qua.27018>
11. *Subtle Chemical Changes Cross the Boundary between Agonist and Antagonist: New A3 Adenosine Receptor Homology Models and Structural Network Analysis Can Predict This Boundary*. Yoonji Lee, Xiyan Hou, Jin Hee Lee, Akshata Nayak, Varughese Alexander, Pankaz K. Sharma, Hyerim Chang, Khai Phan, Zhan-Guo Gao, Kenneth A. Jacobson, Sun Choi and Lak Shin Jeong, *J. Med. Chem.*, **2021**, 64,12525–12536 <https://doi.org/10.1021/acs.jmedchem.1c00239>
12. *Unsupported Donor–Acceptor Complexes of Noble Gases with Group 13 Elements*. Lakhya J. Mazumder, Amlan J. Kalita, Shahnaz S. Rohman, Chayanika Kashyap, Sabnam S. Ullah, Indrani Baruah, Ashapurna Boro, Ankur K. Guha and Pankaz K. Sharma, *ACS Omega*, **2021**, 6, 8656–8661. <https://doi.org/10.1021/acsomega.1c00543>
13. *A Physiological Examination of the Antioxidant Ability of Super Tocopherol Derivatives*. Lakhya J. Mazumder, Pankaz K. Sharma and Ankur K. Guha, *Struct. Chem.*, **2020**, 31, 2313–2319. <https://doi.org/10.1007/s11224-020-01585-x>
14. *Ultra-Weak Metal–Metal Bonding: Is There a Beryllium-Beryllium Triple Bond?* Shahnaz S. Rohman, Chayanika Kashyap, Sabnam S. Ullah, Ankur K. Guha, Lakhya J. Mazumder and Pankaz K. Sharma *ChemPhysChem*, **2019**, 20, 516-518. <https://doi.org/10.1002/cphc.201900051>

15. *Al(He)N³⁺ Clusters: A Theoretical Study*. Sabnam S. Ullah, Chayanika Kashyap, Ankur Kanti Guha, Apurba Kr. Barman, Alok Ch. Kalita and Pankaz K. Sharma, *Curr. Sci.*, **2018**, *114*, 2138-2142. <http://dx.doi.org/10.18520/cs/v114/i10/2138-2142>
16. *Donor Stabilized Borylnitrenes: A Theoretical Study*. Sabnam S. Ullah, Pankaz K. Sharma, and Ankur K. Guha, *Comput. Theor. Chem.*, **2017**, *1115*, 307-312. <https://doi.org/10.1016/j.comptc.2017.07.011>
17. *Electronic Structure, Stability, and Aromaticity of H₂B₂XH (X=N, P) Molecules: A Theoretical Study*. Sabnam S. Ullah, Lakhya J. Mazumder, Samhita Kaushik, Navanita Das, Mainao S. Brahma, Pankaz K. Sharma, and Ankur K. Guha, *Comput. Theor. Chem.*, **2017**, *1113*, 120-125. <https://doi.org/10.1016/j.comptc.2017.05.007>
18. *Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction*. Anna Lopata, Pablo G. Jambrina, Pankaz K. Sharma, Bernard R. Brooks, Judit Toth, Beata G. Vertessy, and Edina Rosta; *ACS Catal.*, **2015**, *5*, 3225–3237. <https://doi.org/10.1021/cs502087f>
19. *Transient Receptor Potential Vanilloid Type 1 Antagonists: A Patent Review (2011 - 2014)*. Yoonji Lee, Sunhye Hong, Minghua Cui, Pankaz K. Sharma, Jeewoo Lee and Sun Choi; *Expert Opin. Ther. Pat.*, **2015**, *25*, 291-318. <https://doi.org/10.1517/13543776.2015.1008449>
20. *2-Aryl Substituted Pyridine C-region Analogues of 2-(3-Fluoro-4-methyl sulfonylaminophenyl) propanamides as Highly Potent TRPV1 Antagonists*. Hyung Chul Ryu, Sejin Seo, Myeong Seop Kim, Kim Mi-Yeon, Ho Shin Kim, Jihae Ann, Phuong-Thao Tran, Van-Hai Hoang, Jieun Byun, Minghua Cui, Karam Son, Pankaz K. Sharma, Sun Choi, Peter M. Blumberg, Robert Frank-Foltyn, Gregor Bahrenberg, Babette-Yvonne Koegel, Thomas Christoph, Sven Frommann, Jeewoo Lee, *Bioorg. Med. Chem. Lett.*, **2014**, *24*, 4044-4047. <https://doi.org/10.1016/j.bmcl.2014.05.072>
21. *2-Alkyl/Alkenyl Substituted Pyridine C-region Analogues of 2-(3-Fluoro-4-methylsulfonylaminophenyl)propanamides as Highly Potent TRPV1 Antagonists*. Hyung Chul Ryu, Sejin Seo, Seong-Hee Cho, Ho Shin Kim, Dong Wook Kang, Karam Son, Minghua Cui, Sun-hye Hong, Pankaz K. Sharma, Sun Choi, Peter M. Blumberg, Robert Frank-Foltyn, Gregor Bahrenberg, Hannelore Stockhausen, Klaus Schiene, Thomas Christoph, Sven Frommann, Jeewoo Lee, *Bioorg. Med. Chem. Lett.*, **2014**, *24*, 4039-4043. <https://doi.org/10.1016/j.bmcl.2014.05.074>
22. *Why Nature Really Chose Phosphate*. Shina C. L. Kamerlin, Pa K. Sharma, Ram B. Prasad, and Arie Warshel (Review article) *Quart. Rev. Biophys.*, **2013**, *46*, 1-132. <https://doi.org/10.1017/S0033583512000157>
23. *Ketosteroid Isomerase Provides Further Support for the Idea that Enzymes Work by Electrostatic Preorganization*. Shina C. L. Kamerlin, Pankaz K. Sharma, Zhen T. Chu and Arie Warshel; *Proc. Natl. Acad. Sci. USA*, **2010**, *107*, 4075-4080. <https://doi.org/10.1073/pnas.0914579107>
24. *Electrostatic Basis for the Unidirectionality of the Primary Proton Transfer in Cytochrome c Oxidase*. Andrei V. Pisliakov, Pankaz K. Sharma, Zhen T. Chu, Maciej Haranczyk and Arie Warshel; *Proc. Natl. Acad. Sci. USA*, **2008**, *105*, 7726-7731. <https://doi.org/10.1073/pnas.0800580105>
25. *The Energetics of the Primary Proton Transfer in Bacteriorhodopsin Revisited: It is a Sequential Light Induced Charge Separation After All*. Sonja Braun-Sand, Pankaz K Sharma, Zhen T Chu, Andrei V Pisliakov and Arie Warshel; *Biochim. Biophys. Acta – Bioenergetics*, **2008**, *1777*, 441-452. <https://doi.org/10.1016/j.bbabi.2008.03.001>
26. *A New Paradigm for Electrostatic Catalysis of Radical Reactions in Vitamin B12 Enzymes*. Pankaz K. Sharma, Zhen T. Chu, Mats H. M. Olsson and Arie Warshel, *Proc. Natl. Acad. Sci., USA*, **2007**, *104*, 9661-9666. <https://doi.org/10.1073/pnas.0702238104>
27. *Electrostatic Contributions to Binding of Transition State Analogues can be Very Different from the Corresponding Contributions to Catalysis: Phenolates Binding to the Oxyanion Hole of Ketosteroid Isomerase*. Arie Warshel, Pankaz K. Sharma, Zhen T. Chu and Johan Åqvist; *Biochemistry*, **2007**, *46*, 1466-1476. <https://doi.org/10.1021/bi061752u>
28. *Modeling Electrostatic Effects in Proteins*. Arie Warshel, Pankaz K. Sharma, Mitsunori Kato and William W. Parson, *Biochim. Biophys. Acta*, **2006**, *1764*, 1647–1676. <https://doi.org/10.1016/j.bbapap.2006.08.007>
29. *Electrostatic Basis for Enzyme Catalysis*. Arie Warshel, Pankaz K. Sharma, Mitsunori Kato, Yun Xiang, Hanbin Liu, and Mats H. M. Olsson, *Chem. Rev.*, **2006**, *106*, 3210-3235. <https://doi.org/10.1021/cr0503106>
30. *Ferromagnetic Bonding: High Spin Copper Clusters (ⁿ⁺¹Cu_n; n = 2-14) Devoid of Electron Pairs but Possessing Strong Bonding*. Samuël P. de Visser, Devesh Kumar, Mark Danovich, Nir Nevo, David

- Danovich, Pankaz K. Sharma, Wei Wu, and Sason Shaik; *J. Phys. Chem. A.*, **2006**, *110*, 8510-8518. <https://doi.org/10.1021/jp055125a>
31. *What Are the Roles of Substrate-Assisted Catalysis and Proximity Effects in Peptide Bond Formation By the Ribosome?* Pankaz K. Sharma, Yun Xiang, Mitsunori Kato and Arieh Warshel, *Biochemistry*, **2005**, *44*, 11307-11314. <https://doi.org/10.1021/bi0509806>
 32. *Sulfoxidation Mechanisms Catalyzed by Cytochrome P450 and Horseradish Peroxidase Models: Spin Selection Induced by the Ligand.* Devesh Kumar, Samuël P. De Visser, Pankaz K. Sharma, Hajime Hirao and Sason Shaik, *Biochemistry*, **2005**, *44*, 8148-8158. <https://doi.org/10.1021/bi050348c>
 33. *Simulating Redox Coupled Proton Transfer in Cytochrome c Oxidase; Looking for the Proton Bottleneck.* Mats H. M. Olsson, Pankaz K. Sharma and Arieh Warshel, *FEBS Lett.*, **2005**, *579*, 2026-2034. <https://doi.org/10.1016/j.febslet.2005.02.051>
 34. *The Intrinsic Axial Ligand Effect on Propene Oxidation by Horseradish Peroxidase versus Cytochrome P450 Enzymes.* Devesh Kumar, Samuël P. de Visser, Pankaz K. Sharma, Etienne Derat and Sason Shaik, *J. Biol. Inorg. Chem.*, **2005**, 181-189. <https://doi.org/10.1007/s00775-004-0622-4>
 35. *Porphyrin Traps Own Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450.* Pankaz K. Sharma, Rouslan Kevorkiants, Samuël P. de Visser, Devesh Kumar and Sason Shaik, *Angew. Chem. Int. Ed.*, **2004**, *43*, 1129 – 1132. <https://doi.org/10.1002/anie.200352943>
 36. *Radical Clock Substrates, their C-H Hydroxylation Mechanism by Cytochrome P450 and Other Reactivity Patterns: What Does Theory Reveal About the Clocks' Behavior?* Devesh Kumar, Samuël P. de Visser, Pankaz K. Sharma, Shimrit Cohen and Sason Shaik, *J. Am. Chem. Soc.*, **2004**, *126*, 1907– 1920. <https://doi.org/10.1021/ja039439s>
 37. *The “Rebound Controversy”: An Overview and Theoretical Modeling of the Rebound Step in Mono-Oxygenation by Cytochrome P450.* Sason Shaik, Shimrit Cohen, Samuël P. de Visser, Pankaz K. Sharma, Sebastian Kozuch, Devesh Kumar, François Ogliaro and David Danovich, *Eur. J. Inorg. Chem.*, **2004**, 207-226. <https://doi.org/10.1002/ejic.200300448>
 38. *Active Species of Horseradish Peroxidase (HRP) and Cytochrome P450: Two Electronic Chameleons.* Samuël P de Visser, Sason Shaik, Pankaz K. Sharma, Devesh Kumar and Walter Thiel, *J. Am. Chem. Soc.*, **2003**, *125*, 15779-15788. <https://doi.org/10.1021/ja0380906>
 39. *Can a Single Oxidant with Two Spin States Masquerade as Two Different Oxidants? A Study of the Sulfoxidation Mechanism by Cytochrome P450.* Pankaz K. Sharma, Samuël P. de Visser and Sason Shaik, *J. Am. Chem. Soc.*, **2003**, *125*, 8698-8699. <https://doi.org/10.1021/ja035135u>
 40. *Science: Viewing La Vega.* Pankaz K. Sharma and Sason Shaik, *Angew. Chem. Int. Ed.* **2003**, *42*, 968; (*Wissenschaft: Viva La Vega*, *Angew. Chem.* **2003**, *115*, 998.) <https://doi.org/10.1002/anie.200390278>
 41. *Is the Ruthenium Analog of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction.* Pankaz K. Sharma, Samuël P. de Visser, François Ogliaro, and Sason Shaik, *J. Am. Chem. Soc.*, **2003**, *125*, 2291-2300. <https://doi.org/10.1021/ja0282487>
 42. *What Factors Affect the Regioselectivity of Oxidation by Cytochrome P450? A DFT Study of Allylic Hydroxylation and Double Bond Epoxidation in a Model Reaction.* Samuël P. de Visser, François Ogliaro, Pankaz K. Sharma and Sason Shaik, *J. Am. Chem. Soc.*, **2002**, *124*, 11809-11826. <https://doi.org/10.1021/ja026872d>
 43. *Hydrogen Bonding Modulates the Selectivity of Enzymatic oxidation by P450: Chameleon Oxidant Behavior by Compound I.* Samuël P de Visser, François Ogliaro, Pankaz K. Sharma and Sason Shaik, *Angew. Chem. Int. Ed.*, **2002**, *41*, 1947-1951. <https://doi.org/10.1002/1521-3773>
 44. *Searching for the Second Oxidant in the Catalytic Cycle of Cytochrome P450: A Theoretical Investigation of the Iron(III)-Hydroperoxo Species and its Epoxidation Pathways.* François Ogliaro, Sam P. de Visser, Shimrit Cohen, Pankaz K. Sharma and Sason Shaik, *J. Am. Chem. Soc.*, **2002**, *124*, 2806-2817. <https://doi.org/10.1021/ja0171963>
 45. *A Theoretical Study of Transition Metal Complexes of C60 and C70 and their Ring-opened Alternatives.* Eluvathingal D. Jemmis and Pankaz K. Sharma, *J. Mol. Graph. Model*, **2001**, *19*, 256- 265. [https://doi.org/10.1016/S1093-3263\(00\)00091-7](https://doi.org/10.1016/S1093-3263(00)00091-7)
 46. *Aza-bowls: Synthesis and Molecular Structure of Triaza-[3]-Peristylane.* Goverdhan Mehta, Ramdas Vidya, Pankaz K. Sharma and Eluvathingal D. Jemmis, *Tet. Lett.*, **2000**, *41*, 2999-3002. [https://doi.org/10.1016/S0040-4039\(00\)00291-4](https://doi.org/10.1016/S0040-4039(00)00291-4)

47. *Exohedral η^5 - and η^6 -Transition Metal Organometallic Complexes of C₆₀ and C₇₀: A Theoretical Study.* Eluvathingal D. Jemmis, Mariappan Manoharan and Pankaz K. Sharma, *Organometallics*, **2000**, 19, 1879-1887. <https://doi.org/10.1021/om9905355>
48. *[n]-Peristylenes and [n]-Oxa-[n]-Peristylenes (n = 3-6): A Theoretical Study.* Pankaz K. Sharma, Eluvathingal D. Jemmis, Ramdas Vidya and Goverdhan Mehta, *J. Chem. Soc. Perkin Trans.*, **1999**, 257-262 <https://doi.org/10.1039/A806955G>

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Google Scholar Profile: <https://scholar.google.com/citations?user=XNoyGUwAAAAJ>

Web of Science Profile: <https://www.webofscience.com/wos/author/record/JAC-2994-2023>

Scopus Profile: <https://www.scopus.com/authid/detail.uri?authorId=8664891400>

ResearchGate Profile: <https://www.researchgate.net/profile/Pankaz-Sharma>

Invited International Lectures

- 1) **Computational Chemistry and Enzyme Catalysis**; Pankaz K. Sharma; December, **2013**; Joint Symposium 2013; *Ewha Womans University, Japan Women's University and Ochanomizu University for the Promotion of Education and Research for Women in Science*; Seoul, Korea.

Invited National Lectures

- 1) **Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction**; Pankaz K. Sharma; National Seminar on *Modern Trends in Chemical Sciences*, 2015 organized by Department of Chemistry, Gauhati University, Guwahati (INDIA), 2015.
- 2) **Computational Chemistry in Academia and Industry**; Pankaz K. Sharma; December, **2012**; National Seminar on *Industrial Application of Computational Chemistry*; organized by Sir Syed College, Kerala (INDIA)
- 3) **Introduction to Molecular Orbital and Valence Bond Theories**, Pankaz K. Sharma; December, **2012**; National Seminar on *Advances in Quantum Mechanics*; Organized by the Government College of Engineering, Kannur, Kerala (INDIA)

Talks Delivered at the Institute/Department Level

- 1) **Chemistry for Engineers (The Importance of Chemistry in Engineering)**. Pankaz K. Sharma, November, **2000**, organized by Girijananda Chowdhury Institute of Management and Technology (GIMT), Guwahati, India.
- 2) **Role of Mathematics in Biochemical and Biomolecular Studies**; Pankaz K. Sharma; *DBT Star College Scheme Lecture Series*, organized by the Department of Chemistry, Mangaldai College, Mangaldai (INDIA), 2017.
- 3) **Enzymatic Reactions and Electrostatic Effects**; Pankaz K. Sharma; May **2007**; Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India.
- 4) **A New Paradigm for Electrostatic Catalysis of Radical Reactions in Vitamin B₁₂ Enzymes**; Pankaz K. Sharma; May **2007**; Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India.
- 5) **Electrostatic Effects in Enzymatic Reactions: Radical Reaction of Vitamin B₁₂ Enzymes, and Phenolates Binding to the Oxyanion Hole of Ketosteroid Isomerase**; Pankaz K. Sharma, May **2007**; Department of Chemistry, Indian Institute of Technology, Delhi, India.

Poster Presentations in International Conferences and Symposia

- 1) A new Paradigm for Electrostatic Catalysis of Radical Reactions in Vitamin B₁₂ Enzymes; Pankaz K. Sharma, Zhen T. Chu, Mats H. M. Olsson and Arieh Warshel; in the *Symposium of the Lise Meitner-Minerva Center*, The Hebrew University of Jerusalem, Israel: November, **2008**. http://alpha.ch.huji.ac.il/public_html/Beirat2008/Book_Abstract_2008.pdf P34 (Pages 7, 34).
- 2) Electrostatic Basis for the Unidirectionality of the Primary Proton Transfer in Cytochrome c Oxidase; Andrei V. Pisliakov, Pankaz K. Sharma, Zhen T. Chu, Maciej Haranczyk and Arieh Warshel; in the *Symposium of the Lise Meitner-Minerva Center*, The Hebrew University of Jerusalem, Israel: November, **2008**. http://alpha.ch.huji.ac.il/public_html/Beirat2008/Book_Abstract_2008.pdf P35 (Pages 7, 64).
- 3) Electrostatic Contributions to Binding of Transition State Analogues can be Very Different from the Corresponding Contributions to Catalysis: Phenolates Binding to the Oxyanion Hole of Ketosteroid Isomerase; Arieh Warshel, Pankaz K. Sharma, Zhen T. Chu and Johan Åqvist; in the *20th Enzyme Mechanisms Conference*, St Pete Beach, Florida, USA: January, **2007**. http://www.divbiolchem.org/content/winter_2007.pdf
- 4) What are the Roles of Substrate-Assisted Catalysis and Proximity Effects in Peptide Bond Formation By the Ribosome?; in *Workshop on Multiscale Modeling in Soft Matter and Bio-Physics*; University of California, Los Angeles (UCLA), Los Angeles, USA: September, **2005**. <http://www.ipam.ucla.edu/programs/maws1>
- 5) A Single Oxidant with Two Spin States or Two Different Oxidants? DFT Study of the Sulfoxidation Reaction Mechanism by Cytochrome P450; Pankaz K. Sharma, Samuël P. de Visser and Sason Shaik; The 1st Annual Meeting of the Israeli Theoretical Chemists (*Israel TheoChem 2002*); Jerusalem, Israel: October, **2002**. 94.23.146.173/ficheros/7997ef4d1f3d52986ff6f0a67758341d.pdf (Page 17)
- 6) The Reaction Mechanism of Oxidation of Dimethyl Sulfide by Compound I of Cytochrome P450. A Density Functional Study; Pankaz K. Sharma, Sam P. de Visser and Sason Shaik; in the *Minerva School in Computational Quantum Chemistry*; Blankensee, Berlin, Germany: September, **2002**. http://alpha.ch.huji.ac.il/public_html/school-berlin/Abstracts/Abs-Post-PK.Sharma1.pdf
- 7) Is the Ruthenium Analog of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction; Pankaz K. Sharma, Sam P. de Visser, François Ogliaro, Shimrit Cohen and Sason Shaik; in the *Minerva School in Computational Quantum Chemistry*, Blankensee, Berlin, Germany: September, **2002**. http://alpha.ch.huji.ac.il/public_html/school-berlin/Abstracts/Abs-Post-PK.Sharma2.pdf
- 8) Is the Ruthenium Analog of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction; Pankaz K. Sharma, Sam P. de Visser, François Ogliaro, Shimrit Cohen and Sason Shaik; in the *67th Annual Meeting of the Israel Chemical Society*, Jerusalem, Israel: January, **2002**. <http://www.chemistry.org.il/ICS/Poster67.htm> (T31)
- 9) Competitive Hydroxylation and Epoxidation Reactions of Cytochrome P450 with Propene. A Density Functional Study; Sam.P. de Visser, Francois. Ogliaro, Pankaz K. Sharma, Sason. Shaik; in the *67th Annual Meeting of the Israel Chemical Society*, Jerusalem, Israel: January, **2002**. <http://www.chemistry.org.il/ICS/Poster67.htm> (T25)
- 10) Is the ruthenium analog of compound I of Cytochrome P450 an efficient oxidant? A theoretical investigation of the methane hydroxylation reaction; Pankaz K. Sharma, Shimrit Cohen, François Ogliaro, and Sason Shaik; in *Electronic Structure: An Interplay of Theory and Experiment*, Hebrew University of Jerusalem in Israel, Jerusalem, Israel: October, **2001** http://alpha.ch.huji.ac.il/public_html/PDFS/Abstracts.pdf (Pages 2, 12)
- 11) [n]-Peristylenes and [n]-Oxa-[n]-Peristylenes (n=3-6): A Theoretical Study; Pankaz K. Sharma, Eluvathingal D. Jemmis, Ramdas Vidya and Goverdhan Mehta; in the *Twelfth International Conference on Computers in Chemical Research and Education (ICCCRE XII)*; Pune, India: January, **1998**. <http://www.t.soka.ac.jp/chem/acen/ICCCRE12.html>

Poster Presentations in National Conferences and Symposia

- 1) [n]-Peristylenes and [n]-Oxa-[n]-Peristylenes (n=3-6): A Theoretical Study, Pankaz K. Sharma, Eluvathingal D. Jemmis, Ramdas Vidya and Goverdhan Mehta, in *Theoretical Chemistry Symposium 1998*, December **1998**, University of Hyderabad, Hyderabad, India
- 2) Classical versus Nonclassical Bonding in XB₃H₃, X = N, CH, P, SiH, BH⁺:Nucleus Independent Chemical Shift (NICS) studies at HF, MP2 and B3LYP levels; Pankaz K. Sharma and Eluvathingal D. Jemmis; in *Modern Trends in Main Group Chemistry*, March, **1997**; Indian Institute of Technology, Delhi, India.

Participation in International Conferences

- 1) **2014 KSBMB Annual Meeting**, Korean Society for Biochemistry and Molecular Biology, May, **2014**; Seoul, Korea.
- 2) **WCI-BP 2013 Korea: The 4th World Class Institute and Brain Pool Symposium**, November, **2013**; Seoul, Korea.
- 3) **2013 Fall International Convention of the Pharmaceutical Society of Korea**, October, **2013**; Osong, Korea.
- 4) **ABA Jeju 2013: 8th Asian Biophysics Association (ABA) Symposium**, May **2013**; Jeju Island, Korea
- 5) **Frontiers in the Simulation of Macromolecules**, November **2010**; Los Angeles, CA, USA.
(<http://michele.usc.edu/FSM2010/participants.html>)

Participation in International Conferences

- 1) **2014 KSBMB Annual Meeting**, Korean Society for Biochemistry and Molecular Biology, May, **2014**; Seoul, Korea.
- 2) **WCI-BP 2013 Korea: The 4th World Class Institute and Brain Pool Symposium**, November, **2013**; Seoul, Korea.
- 3) **2013 Fall International Convention of the Pharmaceutical Society of Korea**, October, **2013**; Osong, Korea.
- 4) **ABA Jeju 2013: 8th Asian Biophysics Association (ABA) Symposium**, May **2013**; Jeju Island, Korea
- 5) **Frontiers in the Simulation of Macromolecules**, November **2010**; Los Angeles, CA, USA.
(<http://michele.usc.edu/FSM2010/participants.html>)

Workshops Conducted

- 1) **The Extended Hückel Theory—A Hands-on Workshop on Its Utility and Limitations**; Pankaz K. Sharma; at the *Lise Meitner–Minerva Center for Computational Quantum Chemistry*, Hebrew University of Jerusalem, Israel; June, **2002**. http://alpha.ch.huji.ac.il/public_html/PDFS/Bairat-2002-Full-report.pdf (Page 14).

Workshops/Schools Attended

- 1) **Multiscale Modeling in Soft Matter and Bio-Physics**; University of California, Los Angeles (UCLA), Los Angeles, USA: September, **2005**
- 2) **Minerva School on Theoretical Chemistry**, September 24–28, **2002**, held in Berlin, Germany.
- 3) **Second Winter School on Theoretical Chemistry (Statistical Mechanics)**, held at the Indian Institute of Technology (IIT) Kanpur (India) during February. 6–26, **2000**; conducted by the Scientific and Engineering Research Council (SERC), Department of Science and Technology, Government of India.
- 4) **First winter school on Theoretical Chemistry (Quantum Chemistry)**, held at the Indian Institute of Technology (IIT) Bombay, Mumbai (India), and the National Chemical Laboratory (NCL), Pune (India), December 3–23, **1998**; conducted by the Scientific and Engineering Research Council (SERC), Department of Science and Technology, Government of India.

Mentoring

- 1) Tutored two undergraduate students and supervised their work for **2002** (Fall) **2003** (Spring) and **2003** (Fall) on the basics of computational chemistry semesters at the Hebrew University of Jerusalem, Israel. http://alpha.ch.huji.ac.il/public_html/PDFS/Bairat-2002-Full-report.pdf (Page 33).

Awards/Fellowships

- Brain Pool invited researcher, Korean Federation of Science and Technology (April 2013 – March 2013)
- Senior Research Fellowship, Council of Scientific and Industrial Research, Govt. of India (1997–2000)
- Junior Research Fellowship, Council of Scientific and Industrial Research, Govt. of India (1995–1997)
- Qualified in the Graduate Aptitude Test for Engineers (GATE), India (1995).
- National Merit Scholarship, Government of India (1986–1991)
- State Merit Scholarship, Government of Assam, India (1986–1994)