

## **Pankaz K. Sharma**

Associate Professor

Department of Chemistry

Cotton College State University (CCSU)

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### **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: ***Professor E. D. Jemmis***
- M.Sc. (Physical Chemistry) University of Delhi, India (1995)  
B.Sc. (Major: Chemistry) Gauhati University, India (1991)

### **Employment History**

- 1) Associate Professor in Chemistry, Cotton College State University, 2015- Present
- 2) Research Professor/Brain Pool Researcher (2013-2014)  
**College of Pharmacy and School of Pharmaceutical Sciences, Ewha Womans University, Seoul**
- 3) Assistant Professor in Computational Sciences (Guest Faculty)  
**Department of Chemistry, Sir Syed College, Kerala (2012)**
- 4) Research Associate (2008 – 2012); Postdoctoral Research Associate (2003 – 2008)  
**Department of Chemistry, University of Southern California**  
Supervisor: ***Professor Arieh Warshel***, USC Distinguished Professor (**Nobel Prize in Chemistry, 2013**)
- 5) Postdoctoral Fellow (2001–2003)  
**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

### **Areas of Expertise**

- Applied Theoretical (Computational Quantum) Chemistry
- Computational Biophysics/Biochemistry
- Computational Bioinorganic Chemistry

### **Professional Experience**

#### **Grant Applications for External Funding**

- Assisted Professor Arieh 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.

- 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)

## Selected Peer-Reviewed Research Publications

Hirsch (H) Index = 22

- 1) *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.
- 2) *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, 291-331.
- 3) *Why Nature Really Chose Phosphate.* Shina C. L. Kamerlin, Pankaz K. Sharma, Ram B. Prasad, and Arieh Warshel; *Quart. Rev. Biophys.*, **2013**, 1-132.
- 4) *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 Arieh Warshel; *Proc. Natl. Acad. Sci. USA*, **2010**, 107, 4075-4080.
- 5) *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; *Proc. Natl. Acad. Sci. USA*, **2008**, 105, 7726-7731.
- 6) *A New Paradigm for Electrostatic Catalysis of Radical Reactions in Vitamin B<sub>12</sub> Enzymes.* Pankaz K. Sharma, Zhen T. Chu, Mats H. M. Olsson and Arieh Warshel, *Proc. Natl. Acad. Sci., USA*, **2007**, 104, 9661-9666.
- 7) *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; *Biochemistry*, **2007**, 46, 1466-1476.
- 8) *Modeling Electrostatic Effects in Proteins.* Arieh Warshel, Pankaz K. Sharma, Mitsunori Kato and William W. Parson, *Biochim. Biophys. Acta*, **2006**, 1764, 1647–1676.
- 9) *Electrostatic Basis for Enzyme Catalysis.* Arieh Warshel, Pankaz K. Sharma, Mitsunori Kato, Yun Xiang, Hanbin Liu, and Mats H. M. Olsson, *Chem. Rev.*, **2006**, 106, 3210-3235.
- 10) *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.
- 11) *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.
- 12) *Porphyrim 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.
- 13) *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.
- 14) *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.)
- 15) *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.
- 16) *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.
- 17) *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.
- 18) *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.

- 19) *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.

### Invited International and National 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).
- 2) *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.
- 3) *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)
- 4) *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)

### 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.

### Awards/Fellowships

- Brain Pool invited researcher, Korean Federation of Science and Technology (April 2013 – March 2014)
- 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)

### Courses Taught at CCSU:

Undergraduate	Post-Graduate
CHM101C (Physical Chemistry I): Unit 3	CHM701C (Physical Chemistry – 1): Unit 4
CHM201C (Physical Chemistry II): Unit 2	CHM801C (Physical Chemistry – 2): Unit 3
CHM301C (Physical Chemistry III): Unit 3	CHM902C (Molecular Spectroscopy- 1): Units 3 -4
CHM401C (Physical Chemistry IV); Unit 2	CHM1213E (Advanced Quantum Chemistry): Units 2-3
CHM501C (Quantum Chemistry): Unit 2	CHM1001C (Quantum Chemistry): Units 1-2
CHM601C (Molecular Spectroscopy): Unit 3	CHM1002C (Chemical Kinetics & Electrochemistry): Unit 1
	CHM1062C (Bio-Inorganic Chemistry): Units 1-2