

## **Dr. Dandamudi Usharani**

---

Principal Scientist, FS&AQCL  
Central Food Technological Research Institute,  
Council of Scientific and Industrial Research, Mysore  
Karnataka 570 020, India  
E-mail: [ushadandamudi.rani@gmail.com](mailto:ushadandamudi.rani@gmail.com), [ushad@cftri.res.in](mailto:ushad@cftri.res.in)



### **Research Area/Interests**

---

#### **Computational Bioinorganic Chemistry / Biochemistry / Structural Biology, Molecular Modeling, Biocatalysis and Disease Mechanisms**

- Elucidation of the reaction mechanisms in the catalytic cycles of the metalloenzymes and the biomimetic models (Enzyme and Homogeneous Catalysis)
- Understanding the structure-function relationships of the biomolecules, inorganic complexes and organic molecules
- Analysis of the structural basis for protein-ligand interactions for rationalizing the mechanism and designing selectivity (Structure Based Drug Design)
- Understanding the electronic structure, bonding and spectroscopic analysis of the active catalytic species and the organometallic complexes that are of biological interest

### **Research Experience**

---

**Scientist Fellow (Quick Hire Scheme)** 2014-2017  
Department of Lipid Science, CSIR-Central Food Technological Research Institute, Mysore

**Postdoctoral Fellow** 2009-2014  
The Hebrew University of Jerusalem, Givat Ram Campus, Jerusalem, Israel  
**Research Group:** Prof. Sason Shaik

### **Education Qualifications**

---

**Doctor of Philosophy, Computational Chemistry** 2004-2009  
Junior Research Scholar at School of Chemistry, Univ. of Hyd., Hyderabad  
Senior Research Scholar at Dept. of Inorg and Phys. Chem., Ind. Inst. of Sci., Bangalore,  
• **Thesis Advisor:** Prof. E. D. Jemmis  
• **Thesis Title:** Computational Structural Aspects of the Phosphorus Containing Clusters and Phosphodiesterases

**Master of Science, General Chemistry** 1996-1998  
School of Chemistry, Univ. of Hyd., Hyderabad, India **Grade:** First Class (69%)

**Bachelor of Science, Genetics, Zoology, Chemistry** 1993-1996  
Shadan Coll., Osm. Univ., Hyderabad, India **Grade:** First Class with Distinction (86%)

## Teaching Experience

---

- |   |           |
|---|-----------|
| Lecturer, Guntur Vikas Junior College, Hyderabad, India | 2001-2003 |
| Lecturer, Vignan Junior College, Hyderabad, India       | 2000-2001 |
| Lecturer, MNR Degree College, Hyderabad, India          | 1998-2000 |
- Mentored students in understanding the basic concepts of general chemistry
  - Achieved 100% results and provided a rigorous training to achieve good results in competitive Engineering, Agricultural and Medical Common Entrance Test (EAMCET)

## Awards/Honors

---

- Attained 7<sup>th</sup> position at District level in secondary school examination
- **Mrs Vaidehi Kishan Rao Memorial Gold Medal** from Osmania University, B.Sc., 1996
- Qualified CSIR-NET (National Eligibility Test) (2003); CSIR-JRF & SRF (2004-2009)
- Best poster awards in **ACS-CSIR-AOCCB conference-2006** and in **Theoretical Chemistry Symposium-2009** and in **Current Trends in Theoretical Chemistry-2013**
- Selected for Kothari postdoctoral fellowship in 2009

## Scientific Activities

---

### Poster Presentations

- DAE-BRNS symposium on Current Trends in Theoretical Chemistry (CTTC-2013), Bhabha Atomic Research Centre, Mumbai, India
- Recent Advances in Computational Drug Design, IISc, Bangalore, India in 2013
- The 2012 and 2010 Symposium of the Lise Meitner-Minerva Center held at The Hebrew University, Jerusalem, Israel
- 5<sup>th</sup> Schulich Symposium on: Frontiers in Computational Chemistry – Bridging Chemistry and Biology held at Technion-Israel Institute of Technology, Haifa, Israel in 2009
- Discussion Meeting on Theoretical Chemistry (TCS) organized by IISc and JNCASR, Bangalore, India in 2009
- IISc: 100 Years and Beyond. The Indian Institute of Science Centenary Conference held at IISc Campus, Bangalore, India in 2008
- Joint International Conference on Advances in Organic and Chemical Biology (ACS-CSIR-AOCCB 2006), ICT, Hyderabad, India in 2006

### Workshops and Conferences

- Organized International Conference on Computational Modelling of Molecules and Materials” at Nanital, India, October 20<sup>nd</sup>-22<sup>rd</sup>, 2016
- 85<sup>th</sup> Annual Meeting of Society of Biological Chemists (India), at CSIR-CFTRI, Mysore November 2016

- Theoretical Chemistry Symposium (TCS – 2016), University of Hyderabad, Hyderabad, December 2016
- CECAM Workshop on Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond at Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland (Feb 9th –Feb 13th 2015)
- Indo-French Seminar on Women in Science, at Indian Institute of Science, Bangalore, India 2015.
- Scientific Conference on Low Calorie/Non Nutritive Sweeteners: Uses & Safety at Hotel Le Meridien, New Delhi, September 2015
- National Conference on Frontiers in MS Technology and Emerging Applications, at ITC Grand Chola, Chennai, December 2015
- International Symposium on Activation of Dioxygen & Homogeneous Catalytic Oxidation (ADHOC-2012) held at Kibbutz Ramat-Rachel, Jerusalem, Israel
- Modular Course in Cheminformatics, Institute of Bioinformatics and Applied Biotechnology (IBAB), Bangalore, India in 2008
- School on Biomolecular Simulations (SBS), JNCASR, Bangalore, India in 2007
- Drug Design Workshop, IISc, Bangalore, India in 2007
- Workshop on Molecular Modeling and Pharmainformatics at National Institute of Pharmaceutical Education and Research (NIPER), Chandigarh, India in 2004

#### **Invited Talks**

- Regional Centre for Biotechnology, Gurgaon, India, September 2013
- National Institute of Immunology, New Delhi, India, September 2013
- International Institute of Information Technology, Hyderabad, India, September 2013
- For the National Workshop on Primary Computational Methods for Chemical Research (PCMCR) in National Institute of Technology, Warangal, India, September 2013
- CSIR-Indian Institute of Chemical Technology, Hyderabad, India, September 2013
- Department of Biotechnology, University of Hyderabad, India, September 2013
- Central Food and Technological Research Institute, Mysore, India, April 2014
- Tata Institute of Fundamental Research, Mumbai, India, April and November 2014
- 5<sup>th</sup> Symposium on Advanced Biological Inorganic Chemistry (SABIC 2017), at The Stadel, Kolkata, India, January 2017
- 5<sup>th</sup> Modeling of Chemical and Biological (Re) Activity, Indo-German Conference at Turyaa Hotel, Chennai, India, February 2017

#### **Granted Projects**

**2**

- 
- Sponsored project from Vyome Biosciences Pvt. Ltd, New Delhi, India (6.58 lakhs for six months, SSP 210)
  - Consultancy project from Vyome Biosciences Pvt. Ltd, New Delhi, India (6 lakhs per annum)

1. D. Dutta Gupta, D. Usharani, S. Mazumdar, "Mono-nuclear Copper Complexes Mimicking the Intermediates for the Binuclear Copper Center of the Subunit II of Cytochrome Oxidase: A peptide Based Approach", *Dalton Transactions* 2016, 45, 17624 (ISI impact factor 4.177)
2. J. Li, S. Zhou, J. Zhang, M. Schlangen, D. Usharani, S. Shaik, H. Schwarz, "Mechanistic Variants in Gas-phase Metal-oxide Mediated Activation of Methane at Ambient Conditions" *J. Am. Chem. Soc.* 2016, 138, 11368 Selected for *JACS Spotlights* 2016, 138, 12003 (No of Citations: 15, ISI impact factor 11.444).
3. J. Li, S. Zhou, J. Zhang, M. Schlangen, T. Weiske, D. Usharani, S. Shaik, H. Schwarz, "Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations  $[XYO_2]^+$  (X,Y= Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen Atom Transfer. *J. Am. Chem. Soc.* 2016, 138, 7973 (No of Citations: 19, ISI impact factor 11.444).
4. S. Shaik, Chemistry as A Game of Molecular Construction: The Bond-Click Way. (Contributors R. B-K. Wakshlak, D. Usharani, D. A. Sharon) **Book** In Press John Wiley & Sons Inc., 2016. ISBN: 978-1-119-00140-9.
5. D. Usharani, B. Wang, D. A. Sharon, S. Shaik, Principles and Prospects of Spin-States Reactivity in Chemistry and Bioinorganic Chemistry. **Book chapter** in "Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity" Chapter 7, 131-156, 2015, 1<sup>st</sup> Edn, John Wiley & Sons Inc., (Ed., Swart, M., Costas, M.), ISBN:978-1-118-89831-4.
6. D. Mandal, R. Ramanan, D. Usharani, D. Janardanan, B. Wang, S. Shaik "How Does Tunneling Contribute to Counterintuitive C-H Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes? Submitted to *J. Am. Chem. Soc.* 2015, 137, 722 (No of Citations: 35, ISI impact factor 11.444).
7. B. Wang, D. Usharani, C. Li, S. Shaik. "Theory Uncovers an Unusual Mechanism of DNA Repair of a Lesioned Adenine the AlkB Enzymes" *J. Am. Chem. Soc.* 2014, 136, 13895. Selected for *JACS Spotlights* 2014, 136, 14321 (No of Citations: 17, ISI impact factor 11.444).
8. D. Usharani, W. Z. Lai, C. Li, H. Chen, S. Shaik. "A Tutorial for Understanding Chemical Reactivity through Valence Bond Approach." *Chem. Soc. Rev.* 2014, 43, 4968 (ISI impact factor of Journal: 24.892).
9. Y. Yang, W. Bu, D. Usharani, H. Zhang, F. Rwere, S. Im, J. Meagher, M. Tarasev, C. Sun, J. Stuckey, S. Shaik, L. Waskell. "Structural and Functional Characterization of a Cytochrome P450 2B4 F429H Mutant with an Axial Thiolate-Histidine Hydrogen Bond." *Biochemistry*, 2014, 53, 5080 (No of Citations: 3, ISI impact factor of Journal: 3.19).

10. D. Usharani, D. C. Lacy, A. S. Borovik, S. Shaik, "Dichotomous Hydrogen Atom Transfer vs. Proton Coupled Electron Transfer during Activation of X-H Bonds (X = C, N, O) by Nonheme Iron-Oxo Complexes of Variable Basicity." **J. Am. Chem. Soc.**, 2013, 135, 17090 (No of Citations: 85, ISI impact factor of Journal: 11.444).
11. S. Shaik, H. Chen, D. Usharani, W. Thiel, "The QM/MM Approach and Some of Its Applications to Structure and Reactivity of Cytochrome P450 Enzymes." **Book chapter in "Drug Metabolism Prediction"** 2014, 1<sup>st</sup> Edn, John Wiley & Sons Inc., (Ed., J. Kirchmair Series Ed., R. Mannhold, H. Kubinyi, G. Folkers), ISBN:978-3-527-33566-4
12. D. Usharani, D. Janardanan, C. Li, S. Shaik, "A Theory for Bioinorganic Chemical Reactivity of Oxometal Complexes and Analogous Oxidants: The Exchange and Orbital–Selection Rules." **Acc. Chem. Res.**, 2013, 46, 471 (No of Citations: 59, ISI impact factor of Journal: 21.640).
13. Y. Wang, D. Janardanan, D. Usharani, K. Han, L. Que, Jr., S. Shaik. "The Nonheme Iron Oxidant in the Presence of H<sub>2</sub>O<sub>2</sub> and Acetic Acid Is the Cyclic Ferric-peracetate Complex and Not a Perferryl-oxo Complex" **ACS Catalysis**, 2013, 3, 1334 (No of Citations: 47, ISI impact factor of Journal: 5.265).
14. R. Mas-Ballesté, A. R. McDonald, D. Reed, D. Usharani, P. Schyman, P. Milko, S. Shaik, L. Que Jr., "Intramolecular Gas-Phase Reactions in Synthetic Nonheme Oxoiron (IV) Ions: Proximity and Spin-State Reactivity Rules." **Chem. Eur. J.**, 2012, 18, 11747 (No of Citations: 9, ISI impact factor of Journal: 5.925).
15. D. Usharani, C. Zazza, W. Z. Lai. M. Chourasia, L. Waskell, S. Shaik, "A Single-Site Mutation (F429H) converts the Enzyme CYP 2B4 into a Heme Oxygenase: A QM/MM Study." **J. Am. Chem. Soc.**, 2012, 134, 4053 (No of Citations: 28, ISI impact factor of Journal: 11.444).
16. D. Janardanan, D. Usharani, S. Shaik, "The Origins of Dramatic Axial Ligand Effects: Closed-Shell Mn<sup>VO</sup> Complexes Use Exchange-Enhanced Open-Shell States to Mediate Efficient H-Abstraction Reactions." **Angew. Chem., Int. Ed.**, 2012, 51, 4421 (No of Citations: 21, ISI impact factor of Journal: 13.455).
17. D. Usharani, D. Janardanan, S. Shaik, "Does the TauD Enzyme Always Hydroxylate Alkanes, While an Analogous Synthetic Non-Heme Reagent Always Desaturates Them?" **J. Am. Chem. Soc.**, 2011, 133, 176 (No of Citations: 32, ISI impact factor of Journal: 11.444).
18. S. Shaik, P. Milko, P. Schyman, D. Usharani, H. Chen, "Trends in Aromatic Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes: A Valence Bond Modeling." **J. Chem. Theory and Comp.**, 2011, 7, 327 (No of Citations: 20, ISI impact factor of Journal: 5.215).
19. D. Janardanan, D. Usharani, H. Chen, S. Shaik, "Modeling C–H Abstraction Reactivity of Nonheme Fe(IV)O oxidants with Alkanes: What Role Do Counter Ions Play?" **J. Phys. Chem. Lett.**, 2011, 2, 2610 (No of Citations: 40, ISI impact factor of Journal: 6.213).

20. P. Schyman, D. Usharani, Y. Wang, S. Shaik, "Brain Chemistry: How Does P450 Catalyze the O-Demethylation Reaction of 5-Methoxytryptamine to Yield Serotonin?" **J. Phys. Chem. B.**, 2010, 114, 7078 (No of Citations: 21, ISI impact factor of Journal: 3.696).
21. K. H. K. Reddy, D. Usharani, J. F. Nixon, E. D. Jemmis, "Structure and Bonding in Stannadiphospholes and their Dianions  $\text{SnC}_2\text{P}_2\text{R}_2^m$  (R=H, *t*Bu  $m=0, -2$ ): A Comparative Study with  $\text{C}_5\text{H}_5^+$  and  $\text{C}_5\text{H}_5^-$  Analogues." **Chem.- Eur. J.**, 2011, 17, 9142 (No of Citations: 1, ISI impact factor of Journal: 5.925).
22. D. Usharani, A. Poduska, J. F. Nixon, E. D. Jemmis, "Electronic Structure and Bonding in Neutral and Dianionic Boradiphospholes:  $\text{R}'\text{BC}_2\text{P}_2\text{R}_2$  (R= H, *t*Bu, R'=H, Ph)." **Chem.- Eur. J.**, 2009, 15, 8429 (No of Citations: 4, ISI impact factor of Journal: 5.925).
23. S. Ghosh, D. Usharani, S. De, E. D. Jemmis, S. Bhattacharya, "Photophysical and Duplex-DNA-Binding Properties of Distamycin Dimers Based on 4,4'- and 2,2'-Dialkoxyazobenzenes as the Core." **Chem. An Asian J.**, 2008, 3, 1949 (No of Citations: 10, ISI impact factor of Journal: 4.572).
24. S. Ghosh, D. Usharani, A. Paul, S. De, E. D. Jemmis, S. Bhattacharya, "Design, Synthesis, and DNA Binding Properties of Photoisomerizable Azobenzene-Distamycin Conjugates: An Experimental and Computational Study." **Bioconj. Chem.**, 2008, 19, 2332 (No of Citations: 14, ISI impact factor of Journal: 4.930).
25. P. Srivani, D. Usharani, E. D. Jemmis, G. Narahari Sastry, "Subtype Selectivity in Phosphodiesterase 4 (PDE4): A Bottleneck in Rational Drug Design." **Curr. Pharma. Design**, 2008, 14, 3854 (No of Citations: 43, ISI impact factor of Journal: 4.774).
26. D. Usharani, P. Srivani, G. Narahari Sastry, E. D. Jemmis, "pH Dependence of a  $3_{10}$ -Helix versus Turn in the M-loop Region of PDE4: Observations on PDB Entries and an Electronic Structure Study." **J. Chem. Theory and Comp.**, 2008, 4, 974 (No of Citations: 3, ISI impact factor of Journal: 5.215).
27. D. Usharani, D. L. V. K. Prasad, J. F. Nixon, E. D. Jemmis, "Electronic Structure and Bonding Studies on Triple-Decker Sandwich Complexes with a  $\text{P}_6$  Middle Ring." A Special Issue "90 years of Chemical Bonding" **J. Comput. Chem.**, 2007, 28, 310 (No of Citations: 3, ISI impact factor of Journal: 4.583).