Manoj Kumar

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**EDUCATION & PROFESSIONAL EXPERIENCE**

* **Post-Doc**, **Computational Atmospheric Chemistry, University of Nebraska-Lincoln, Lincoln, NE, USA June, 2015-present.**

Project title: “Computational Modeling of Atmospheric Chemistry” (with Prof. J. S. Francisco)

* **Post-Doc**, **Computational organometallic Chemistry, University of Kansas, Lawrence, KS, USA May, 2012-May, 2015.**

Project title: “Molecular Modeling of Olefin Ozonolysis” (with Prof. W. H. Thompson) and

“Molecular Modeling of Rhodium-catalyzed Hydroformylation” (with Prof. T. A. Jackson)

* **PhD, Computational Bioinorganic Chemistry, University of Louisville, Louisville, KY, USA 2007-12**

Thesis title: “Computational Modelling of Cobalamin-Dependent Enzymatic Reactions” (with Prof. P. M Kozlowski)

* **Summer Research Project, Computational Material Chemistry, Jawahar Lal Nehru Center for Advanced Scientific Research (JNCASR), Bangalore, India, May,2005-July,2005**

Thesis title: “Theoretical Analysis of Gold Clusters and Their Interactions with Thiolates” (with Prof. Swapan K. Pati)

* **MSc, Computational Material Chemistry, Panjab University, Chandigarh, India, 2004-06**

Thesis title: “Theoretical Analysis of Finite-Sized Gold Clusters” (with Prof. T. K. Sau)

* **BSc, Physics, Chemistry & Mathematics, SVSD PG College, Bhatoli, Himachal Pradesh** **University, Shimla, India, 2001-04**.

**RESEARCH HIGHLIGHTS**

* Successfully reproduced the experimental trends in hydroformylation regioselectivity, which has been a significant challenge, and have shown that the dispersion interactions involving the ligands and substrate, but not the commonly perceived intraligand interactions play a vital role in governing the hydroformylation regiochemistry. Hydroformylation is one of the most commonly used homogenous catalytic processes for the industrial production of aldehydes and their derivatives.
* Provided the first electronic structure evidence about the role of acid catalysis in enhancing the rate of unimolecular and bimolecular Criegee reactions, and carbonic acid decomposition. These reactions have not only received renewed attention as a means to break down long chain biomass molecules into more useful renewable chemical intermediates, but is also relevant in atmospheric chemistry.
* Classified Human Toll-like Receptors as possible drug compounds, solely using the calculated electrostatic potential maps.
* Our computational modeling of the reactivation cycle of methyltransferases, which are important enzymes because their malfunctioning causes cadiovascular risks, neural defects and alzheimer’s disease, has predicted the existence of a new kind of interaction between the Co(I) ion of cob(I)alamin and its axial ligands (Co1+–H interaction).
* Computationally provided an unambiguous solution to Co2+/Co1+ reduction, a common chemical event in a large class of methyltransferases and ATP:Co(I)rrinoid adenosyltransferases.
* Provided the first computational evidence for why hydroxocobalamin, a vitamin B12 analogue with tremendous potential for DNA damage, can be photodissociated in nature.
* Based on electronic structure calculations, we developed a mechanism for the cobalt-carbon bond activation in B12-dependent enzymes. These cobalt-containing enzymes constitute an important subgroup of metalloenzymes that are involved in the carbon cycle, and are biomedically significant because of their role in Vitamin B12 deficiency.

# FELLOWSHIPS, HONORS AND AWARDS

* Invited Speaker, International Conference on Organic Chemistry, Las Vegas, USA, Aug,10-11, 2016.
* Invited Speaker for the session “*Quantum Mechanics Applied to Biophysical Problems*”, American Physical society, March Meeting 2014, Denver, Colorado.
* Invited Speaker, DyMERS Seminar Series, Department of Chemistry, University of Kansas, 4th Sept-2012
* CONTRIBUTED TALK” Travel Award, CBSB12 workshop, University of Tennessee, Knoxville, June 3-5, 2012 (declined due to schedule conflict).
* University of Louisville Graduate Dean’s Citation Award for Excellence in Graduate Studies, May-2012 (This award is given to top 5% of the graduating students).
* University of Louisville, Doctoral Dissertation Completion Award, Spring-2012 (This award is given to the outstanding graduate students in the final semester for the dissertation completion and defense).
* University of Louisville Arts and Sciences Graduate Student Union Fellowship, Feb 2011.
* University of Louisville Arts and Sciences Graduate Student Union Fellowship, Oct 2011.
* National Science Foundation (NSF) Travel Award for attending 4th International Workshop and School “Time-Dependent Density-Functional Theory: Prospects and Applications” Benasque, Spain, 2nd - 15th January, 2010.
* University of California San Diego (UCSD) Travel Award for attending 2009 Center for Theoretical Biophysics (CTBP) Summer School, UCSD, La Jolla, San Diego, 4th - 7th August, 2009.
* University of Louisville Graduate Student Council Travel Award for attending 41st Central Regional Meeting of the ACS, Cleveland, Ohio, 20th - 23rd May, 2009.
* University of Louisville Prestigious Graduate Student Fellowship, fall 2007 - fall 2008.
* Department of Science and Technology (Govt. of India) Award (DST) for attending 18th meeting of “Noble Laureates and Students in Chemistry”, Lindau, Germany, 25th - 30th June, 2006 (Only 26 young Indian researchers from a pool of thousand candidates were selected for attending this meeting).
* Qualified University Grants Commission, Govt. of India, National Eligibility Test (NET), 2006 (This test determine eligibility for college & university level lectureship and for award of Junior Research Fellowship for Indian nationals in order to ensure minimum standards for the entrants in the teaching profession and research).
* Rajiv Gandhi National Talent Research Scholar Award (in the category of Theoretical Sciences), 2005 (This award is given to the top ten Summer Research Projects selected nationwide by JNCASR, Bangalore, India).
* Gold Medalist, Bachelors in Science (BSc) 2004.
* Santosh Shiksha Purskar, 2004 (This award is given to a BSc student who scores the most statewide).
* State Merit Scholarship Award, 1994-1999.
* National Merit Scholarship Award, 1999-2004.

**PUBLICATIONS**

1. P. Lodowski,M. Jaworska, T.Andruniów, **M. Kumar** and P. M. Kozlowski, “Photodissociation of Co-C bond in Methyl- and Ethylcobalamin: An Insight from DFT Calculations”, *J. Phys. Chem. B* **2009**, *113*, 6898-6909.
2. **M. Kumar** and P. M. Kozlowski, “Role of Tyrosine Residue in the Activation of Co-C bond in Coenzyme B12-Dependent Enzymes: Another Case of Proton-Coupled Electron Transfer?”, *J. Phys. Chem. B* **2009**, *113*, 9050-9054.
3. M. Alfonso-Prieto,X. Bairnes, **M. Kumar**, C. Rovira and P. M. Kozlowski, “The Co-C bond cleavage mechanism in cobalamin-dependent methionine synthase: a Theoretical Study”, *J. Phys. Chem. B***2010*,*** *114*, 12965-12971.
4. P. M. Kozlowski,T. Kamachi, **M. Kumar**,T. Nakayama and K. Yoshizawa, “Theoretical Analysis of Diradical Nature of Adenosylcobalamin Cofactor–Tyrosine Complex in B12-Dependent Mutases: Inspiring PCET-driven Enzymatic Catalysis”, *J. Phys. Chem. B* **2010**, *114*, 5928-5939.
5. C. A. Masitas, **M. Kumar**, M. S. Mashuta, P. M. Kozlowski and C. A.Grapperhaus, “Controlled Sulfur Oxygenation of the Ruthenium Dithiolate (bmmp-TASN)RuPPh3 under Limiting O2 Conditions Yields Thiolato/Sulfinato, Sulfenato/Sulfinato, and Bis-Sulfinato Derivatives”, *Inorg. Chem.* **2010,** *49*,10875-10881.
6. N. Kumar, M. Jaworska, P. Lodowski, **M. Kumar** and P. M. Kozlowski, “Electronic Structure of Cofactor-Substrate Reactant Complex Involved in the Methyl Transfer Reaction Catalyzed by Cobalamin-Dependent Methionine Synthase” *J. Phys. Chem. B* **2011***, 115,* 6722-6731*.*
7. P. M. Kozlowski,T. Kamachi, **M. Kumar**,and K. Yoshizawa, “Intial Step of B12-Dependent Enzymatic Catalysis: Energetic Implications Regarding the Involvement of One-Electron Reduced form of Adenosylcobalamin Cofactor”, *J. Biol. Inorg. Chem.* **2011,** *17*, 293-300.
8. **M. Kumar** and P. M. Kozlowski, “A Biologically Relevant Co1+--H Bond: Possible Implications in the Protein-Induced Redox Tuning of Co2+/Co1+ Reduction”*, Angew. Chem. Int. Ed.***2011***,* *50*, 8702-8705.
9. P. M. Kozlowski,T. Kamachi, **M. Kumar** and K. Yoshizawa, “Reductive Elimination Reaction Pathway for Homocysteine to Methionine Conversion in Cobalamin-dependent Methionine Synthase”, *J. Biol. Inorg. Chem.* **2012,** *17*, 611-619.
10. P. M. Kozlowski, **M. Kumar**,P. Piecuch, W. Li, P. Lodowki,and M. Jaworska, “The Co-C Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on DFT, CASSCF/CASPT2 and Completely Renormalized Coupled-Cluster Calculations”, *J. Chem. Theory Comput.* **2012,** *8*, 1870-1894.
11. **M. Kumar** and P. M. Kozlowski, “Why Hydroxocobalamin is photocatalytically active?”, *Chem. Phys. Lett.* **2012**, *543*, 133-136.
12. **M. Kumar**,H. Hirao and P. M. Kozlowski, “Co1+--H Interaction Inspired Alternate Coordination Geometries of Biologically Important Cob(I)alamin: Possible Structural and Mechanistic Consequences for Methyltransferases and ATP:Corrinoid Adenosyltransferases”, *J. Biol. Inorg. Chem.* **2012,** *17***,** 1107-1121.
13. **M. Kumar**,N. Kumar, H. Hirao and P. M. Kozlowski, “Co2+/Co1+ Redox Tuning in Methyltransferases Induced by a Conformational Change at the Axial Ligand”, *Inorg. Chem.* **2012,** *51*, 5533-5538.
14. **M. Kumar** and P. M. Kozlowski, “Corrin Ring-Induced Redox Tuning” *ChemComm* **2012,** *48*, 4456-4458*.*
15. **M. Kumar**, W. Galezowski and P. M. Kozlowski, “Computational Modelling of Electrochemistry of B12 Cofactors”, *Int. J. Quant. Chem.* **2013**, *113*, 479-488.
16. **M. Kumar** and P. M. Kozlowski, “Can The Local Enzyme Scaffold Participate in Co1+--H Bond Formation?: The Curious Case of Methionine Synthase-bound Cob(I)alamin” *J. Inorg. Biochem.* **2013**, *126*, 26-34.
17. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “The Criegee Intermediate Reaction with CO. Mechanism, Barriers, Conformer-Dependence, and Implications for Ozonolysis Chemistry”, *J. Phys. Chem. A* **2014**, *118*, 1887-1894.
18. R. A. Begum, V. W. Day, **M. Kumar**, T. A. Jackson, K. Bowman-James, “M--H-M Interaction. Agostic or Not: A Comparison of Xylyl vs. Pyridyl-Bridged Dimers”, *Inorganica Chim.* *Acta* **2014**, *417*, 287-293.
19. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “Organic Acids Tunably Catalyze Carbonic Acid Decomposition”, *J. Phys. Chem. A* **2014**, *118*, 5020-5028; 10155-10156.
20. **M. Kumar**, R. V. Chaudhari, B. Subramaniamand T. A. Jackson, “Ligand Effects on Regioselectivity of Rhodium-catalyzed Hydroformylation: Density functional calculations illuminate the role of dispersion interactions”, *Organometallics* **2014,** *33*, 4183-4191.
21. Euna Yoo, Deepak B. Salunke, Diptesh Sil, Xiaogiang Guo, Alex C.D. Salyer, Alec R. Hermanson, **Manoj Kumar** et al, “Determinants of Activity at Human Toll-like Receptors 7 and 8: QSAR of Diverse Heterocyclic Scaffolds”, *J. Med. Chem.* **2014**, *57*, 7955-7970.
22. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “Role of Tunable Acid Catalysis in Decomposition of *α*-Hydroxyalkyl Hydroperoxides: Mechanistic Implications for the Atmospheric Formation of Hydrogen Peroxide, Hydroxy Radical and Carbonyl Compounds”, *J. Phys. Chem. A* **2014**, *118*, 9701-9711.
23. **M. Kumar**,D. H. Busch, B. Subramaniamand W. H. Thompson, “Barrierless Tautomerization of a Criegee Intermediate via Acid Catalysis, *Phys. Chem. Chem. Phys.* **2014**, *16*, 22968-22973.
24. **M. Kumar**, R. V. Chaudhari, B. Subramaniamand T. A. Jackson, “Importance of Long-Range Non-Covalent Interactions in the Regioselectivity of Rhodium-Xantphos Catalyzed Hydroformylation”, *Organometallics* **2015**,doi=10.1021**/**om5012775.
25. F. Liu, Y. Fang, **M. Kumar**, W. H. Thompson, M. I. Lester, “Direct Observation of Vinyl Hydroperoxide”, *Phys. Chem. Chem. Phys.* **2015**, *17*, 20490-20494.
26. **M. Kumar**, J. S. Francisco, “The Role of Catalysis in Alkanediol Decomposition: Implications for General Detection of Alkanediols and Their Formation in the Atmosphere”, *J. Phys. Chem. A* **2015**, *119*, 921-9833.
27. **M. Kumar**, J. S. Francisco, “Red-Light-Induced Decomposition of an Organic Peroxy Radical: A New Source of the HO2 Radical”, *Angew. Chem. Int. Ed.***2015***,* *54*, 15711-15714 (**selected for inside back cover**)**.**
28. **M. Kumar**, J. S. Francisco, “Hydrogen Sulfide Induced Carbon Dioxide Activation via Metal Free Dual Catalysis”, *Chem. Eur. J.* **2016**, *22*, 1-6.
29. L. Lei, **M. Kumar**, C. Zhu, J. Zhong, J. S. Francisco, X. C. Zeng, “Near Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton Transfer Mechanism on the Surface of Water Clusters”, *J. Am. Chem. Soc.* **2016**, *138*, 1816-1819 (**Highlights**: C&EN, UNL, Nebraska Center for Material Science and Nanoscience, and USTC (China)).
30. **M. Kumar**, A. Sinha, J. S. Francisco, “Role od Double Hydrogen Atom Transfer Reactions in Atmospheric Chemistry”, *Acc. Chem. Res.* 2016 (being revised).
31. **M. Kumar**, J. S. Francisco, “Red-Light Initiated Bimolecular Decomposition of Hydroxy Methylperoxy Radical: Implications for the HOx Formation in the Troposphere”, submitted to *J. Phys. Chem. A*.
32. **M. Kumar**, J. S. Francisco, “Formation of Elemental Sulfur Aerosols via Hydrogen Sulfide-Selective Catalytic Oxidation”, submitted.

**WORKSHOPS & SUMMER SCHOOLS**

1. Q-Chem Workshop, University of Louisville, Louisville, 30th March, 2010.
2. 4th International Workshop and School “Time-Dependent Density-Functional Theory: Prospects and Applications”, Benasque, Spain, 2nd - 15th January, 2010.
3. CTBP Summer School, UCSD, La Jolla, San Diego, 4th - 7th August, 2009.
4. Q-Chem Workshop, Pittsburgh Supercomputer Center, Pittsburgh, 19th - 20th March, 2009.
5. 18th meeting of “Noble Laureates and Students in Chemistry”, Lindau, Germany, 25th - 30th June, 2006.
6. Summer Research School, JNCASR, Bangalore, India, May - July, 2005.

**PRESENTATIONS**

1. “*Photodissociation of Co-C bond in Methyl- and Ethylcobalamin: An Insight from DFT Calculations*”, Q-Chem Workshop, Pittsburgh Supercomputer Center, Pittsburgh, 19th -20th March, 2009 **(poster)**.
2. “*Photodissociation of Co-C bond in Methyl- and Ethylcobalamin: An Insight from DFT Calculations*” 41st Central Regional Meeting of the ACS, Cleveland, Ohio, 20th - 23rd May, 2009 **(poster)**.
3. “*Role of Tyrosine Residue in the Activation of Co-C bond in Coenzyme B12-Dependent Enzymes: Another Case of Proton-Coupled Electron Transfer?*”, CTBP Summer School, UCSD, La Jolla, San Diego, 4th - 7th August, 2009 **(poster)**.
4. “*Role of Tyrosine Residue in the Activation of Co-C bond in Coenzyme B12-Dependent Enzymes: Another Case of Proton-Coupled Electron Transfer?*”, 4th International Workshop and School “Time-Dependent Density-Functional Theory: Prospects and Applications”, Benasque, Spain, 2nd - 15th January, 2010 **(poster)**.
5. “*The Reductive Cleavage Mechanism of Co-C Bond in Cobalamin-Dependent Methionine Synthase*”, 42nd Central Regional Meeting of the ACS, Dayton, Ohio, 16th – 19th June, 2010 **(poster)**.
6. “*A Biologically Relevant Co1+--H Bond: Possible Implications in the Protein-Induced Redox Tuning of Co2+/Co1+ Reduction*”*,* Graduate Research Symposium, University of Louisville, Louisville, KY, 20th March, 2011 **(oral)**.
7. “*Computational modeling of methyl transfer reactions catalyzed by cobalamin-dependent methionine synthase enzyme*”, 7th Congress of the International Society for Theoretical Chemical Physics, Waseda University, Tokyo, Japan, 2nd – 8th September, 2011 **(oral)**.
8. “*Computational Modeling of Cobalamin-Dependent Methyltransferases*”, Department of Chemistry, University of Kansas, Lawrence, Kansas, 5th Sept., 2012 (**Invited Talk**).
9. “*What factors control the origin of regioselectivity in Rhodium-catalyzed hydroformylation?: DFT offers unprecedented insight*”, Kansas State Physical Chemistry Symposium, Kansas State University, Manhattan, 13th Oct., 2012 **(oral)**.
10. “*What factors control the origin of regioselectivity in Rhodium-catalyzed hydroformylation?: DFT offers unprecedented insight*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 15th-16th Oct., 2012 **(poster)**.
11. “*What factors control the origin of regioselectivity in Rhodium-catalyzed hydroformylation?: DFT offers unprecedented insight*”, Southwest Theoretical Chemistry Conference, College Station, Texas, 26th- 28th Oct., 2012 **(poster)**.
12. “*Direct Observation of Fructosyl Oxocarbenium Ions: Key Intermediates in Biology and Biofuels*”, University of Kansas, Post-Doctoral Research Day, Lawrence, Kansas, 15th March, 2013 **(poster)**.
13. “*DFT Modeling predicts unconventional Mechanistic Pathways for Ozonolysis Reaction*”, National 245th ACS Meeting, New Orleans, Louisiana, 7th-11th April, 2013 **(oral)**.
14. “*Ligand Effects on Regioselectivity in Rhodium-catalyzed hydroformylation: DFT offers Unprecedented Mechanistic Insights*”, National 245th ACS Meeting, New Orleans, Louisiana, 7th-11th April, 2013 **(oral)**.
15. “*Direct Observation of Fructosyl Oxocarbenium Ions: Key Intermediates in Biology and Biofuels*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 15th-16th April, 2013 **(poster)**.
16. “*DFT Modeling predicts unconventional Mechanistic Pathways for Ozonolysis Reaction: Direct Relevance to Industry and Atmosphere*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 15th-16th April, 2013 **(poster)**.
17. “*Non-Covalent Interactions Determine Regioselectivity in Rhodium-catalyzed hydroformylation*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 15th-16th April, 2013 **(poster)**.
18. “*DFT Modeling of Bimolecular Criegee Chemistry*”, National 246th ACS Meeting, Indianapolis, Indiana, 8th-12th Sept., 2013 **(oral)**.
19. “*Non-covalent interactions determine regiochemistry of Rhodium-catalyzed hydroformylation of unsaturated substrates: Another case of B3LYP failure*”, National 246th ACS Meeting, Indianapolis, Indiana, 8th-12th Sept., 2013 **(oral)**.
20. “*DFT Modeling of Olefin Ozonolysis: Direct Relevance to Industry and Atmosphere*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 7th-8th Oct., 2013 **(poster)**.
21. “Molecular Modelling of Regioselectivity of *Rhodium-catalyzed hydroformylation*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 7th-8th Oct., 2013 **(poster)**.
22. “*A Curious Case of Carbonic Acid Decomposition*”, Kansas Physical Chemistry Symposium, University of Kansas, Lawrence, 9th Nov., 2013 **(oral)**.
23. “*Computational Modeling of An Unusual Co(I)--H Interaction: Structural and Mechanistic Ramifications for Cobalamin-Dependent Methyltransferases*”, National American Physics Society Meeting, Denver, Colorado, 3rd-7th March, 2014 (**Invited Talk**).
24. “*Molecular Modeling of α-Hydroxyalkyl Hydroperoxides: Implications for the Selective Formation of Carbonyl Compounds*”, CEBC Annual Industry Board/Annual Scientific Board Meeting, Lawrence, Kansas, 14th-15th April, 2014 **(poster)**.
25. “*Molecular Modeling of Rhodium-Catalyzed Hydroformylation*”, National 248th ACS Meeting, San Francisco, California, 10th-14th Aug., 2014 **(poster under Academic Employment Initiative Program)**.
26. “*Molecular Modeling of Rhodium-Catalyzed Hydroformylation*”, National 248th ACS Meeting, San Francisco, California, 10th-14th Aug., 2014 **(oral)**.
27. “*Molecular Modeling of Carbonic Acid Decomposition*”, National 248th ACS Meeting, San Francisco, California, 10th-14th Aug., 2014 **(oral)**.

**TEACHING EXPERIENCE**

**Fall Term, 2011**: Lecturer, Introduction to Computational Chemistry and Molecular Modeling, an introductory computational quantum Chemistry course for chemistry majors (taught the whole course).

**Spring Term, 2011**: Lecturer, Advanced Physical Chemistry, a graduate-level course in quantum chemistry (presented four 75-minute lectures). Supervised the computational lab project part of Advanced Physical Chemistry course.

**Fall-Summer Term, 2008-11**: Teaching Assistant, Introduction to General Chemistry I, II, Introduction to Chemical Analysis I, II, Elements of Physical Chemistry (for chemistry majors), Physical Chemistry (for chemistry majors), Inorganic Chemistry (for chemistry majors).