

CURRICULUM-VITAE

Dr. DEVESH KUMAR

Professor

Department of Physics

School for Physical and Decision Sciences

Baba Saheb Bhimrao Ambedkar University

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RESEARCH INTEREST

- Studies of the reactivity of organic substrates with metalloenzymes or biomimetic catalysts using quantum chemistry, electronic structure and spectra, quantum mechanics/ molecular mechanics.
- Simulations of intermolecular interactions in mesogens and biological molecules

SUMMARY

- Successfully resolved a controversy that was arisen from different sets of experiments by two research groups on the mechanism of C-H hydroxylation by cytochrome P450 enzymes. Recently, Rittle and Green (Science (2010) 330, 933) characterized the compound I of P450 and found that it perform C-H hydroxylation via rebound mechanism as explained by theory since 2002.
- Explained the role of environment in catalytic reactions of P450 such electric field, water molecule etc.
- Described the oxidation properties of several non-heme enzymes/ systems such as Bleomycin, Cystein Dioxygenase, N4py, Bntpen etc.
- Characterized and suggested several potent oxidants of Polyoxometalate.
- Suggested correlations between physical properties like ionization potential, bond dissociation energies of drug like molecules with reaction barrier of reactions involved in drug metabolism by cytochrome P450 enzymes.

POSITION HOLD:

Aug. 2014 – Present	Professor, Department of Physics, School for Physical and Decision Sciences, Babasaheb Bhimrao Ambedkar University, Lucknow, India
Aug. 2011 – Aug. 2014	Associate Professor, Department of Applied Physics, School for Physical Sciences, Babasaheb Bhimrao Ambedkar University, Lucknow, India

RESEARCH EXPERIENCE

April 2009 – July 2011	Ramanujan Fellow, Indian Institute of Chemical Technology, Hyderabad (A. P.), India Group Leader: Dr. G. Narahari Sastry
June 2006 – March 2009	Postdoctoral Fellow, The Max-Planck-Institut für Kohlenforschung, Mulheim an der Ruhr, Germany Mentor: Professor Walter Thiel

- May 2002 - May 2006 Postdoctoral Fellow, The Hebrew University of Jerusalem, Israel
Mentor: Professor Sason Shaik
- July 2001 - March 2002 Research Associate, Center for Liquid Crystal Research and Education, Nagarjuna University, Nagarjuna Nagar, India
Mentor: Professor V.G.K.M. Pisipati

EDUCATION

- Ph.D., Physics, DDU Gorakhpur University, Gorakhpur, India, 2001
Thesis Title: "*Study of Conformation and Interactions in Mesogens*"
Supervisor: Professor Mihir Roychoudhury
- M.Sc., Physics, University of Gorakhpur, Gorakhpur, India, 1989
- B.Sc., Physics, Chemistry, Mathematics, L. N. Mithla University, Darbhanga, India, 1984

Date of Birth: 5 June 1965

PUBLICATIONS (see list of publications for details):

Review Articles	Five
Research Papers	Eighty Six
Editorials	Two
Book Chapter	Two
Book	One

Journal wise break up:

Journal	IF	No.	Journal	IF	No.
Chem. Rev.	47.928	2	Organometallics	3.862	2
Acc. Chem. Res.	20.268	1	J. Mol. Cat. A	3.679	1
J. Am. Chem. Soc.	13.858	22	J. Chem. Info.Mod.	3.760	1
Angew. Chem. Int. Ed.	11.994	5	Org. Biomolec. Chem.	3.564	1
Nat. Prod. Rep.	11.014	1	Faraday Discuss.	3.558	1
Chemical Science	8.668	1	J. Phys. Chem. B	3.177	4
Chem. Commun.	6.319	3	J. Inog. Biochem.	3.348	2
Chem. Eur. J.	5.317	7	J. Biol. Inorg. Chem.	2.984	3
Inorg. Chem.	4.857	4	Eur. J. Inorg. Chem.	2.942	2
J. Phys. Chem. C	4.536	1	Biochemistry	2.938	1
Phys. Chem. Chem. Phys.	4.123	2	J. Phys. Chem. A	2.847	7
Dalton Transactions	4.029	1	Other Journals	<2	16

Total impact factor	:	640.3
Average impact factor	:	6.9
Citations	:	4436
h-index	:	35
i10-index	:	67

SUPERVISION EXPERIENCE (during PostDoc period; 2002-2009)

PostDoc supervision at the Hebrew University of Jerusalem:

1. Dr. Etienne Derat (2004 – 2005)
2. Dr. Hajime Hirao (2004 – 2005)
3. Dr. Kyung-Bin Cho (2005 – 2006)
4. Dr. Yohann Moreau (2005 – 2006)

PhD student supervision:

1. Chunsen Li (2003 – 2005)
2. Holly N. Frye (2005 – 2006)

Undergraduate student supervision:

1. Tal Katzav (2004 – 2006)
2. Saloni Sahani (2007)

SUPERVISION EXPERIENCE (as Faculty, Aug. 2011 onwards)

	Submitted/Awarded	Working
PhD students :	05	07
MPhil students:	03	00

MAJOR PROJECTS

1. Quantum mechanical/Molecular Mechanics (QM/MM) Studies of the Properties and the Reactivities of Human Isoforms of Cytochrome P450. Cost **Rs. 72.35 lakhs**, sponsored by *Department of Science and Technolgy, New Delhi* for 2009 – 2014.
2. Quantum Mechanical/Molecular Mechanical (QM/MM) studies of the properties and the reactivities of tetrahydropterin-dependent amino acid hydroxylases. **Rs. 37.98 lakhs**, sponsored by *Department of Science and Technolgy, New Delhi* for 2010 – 2013.
3. QM/MM, MD Simulations and Computer Aided Drug Design Approaches on 5-Lipoxygenas, sponsored by *Dst-Conacyt, Mexico S&T Cooperation Programme* for 2011 – 2013.
4. “Molecular Property Diagnostic Suite (MPDS): An OSDD Chemoinformatics Portal” sponsored by *Council of Scientific and Industrial Research, New Delhi* for 2012-13.

ADMINISTRATIVE EXPERIENCE

June 2013 – till date	Director, The University Institute of Engineering & Technology, Babasaheb Bhimrao Ambedkar University, Lucknow
Sept. 2012 – Jan. 2013	Coordinator, NKN of Babasaheb Bhimrao Ambedkar University, Lucknow
Nov. 1999 - July 2001	Research cum Statistical Officer, SC/ST Cell, DDU Gorakhpur University, Gorakhpur, India
Aug. 1995 - Nov. 1999	Coordinator (Computer Courses), Department of Adult, Continuing Education and Extension, DDU Gorakhpur University, Gorakhpur, India

INVITED TALKS

- Refresher Course in Physics, Electronics, Renewable Energy & Information Technology (MD), Lucknow University, March 04, 2014.
- 5th Refresher Course in Physics DDU Gorakhpur University, February 14 - 15, 2014.
- 11th Refresher Course in Chemistry, DDU Gorakhpur University, January 29, 2014.
- Winter School on Modeling Chemical and Biological (Re)activity (MCBR-2014;; Jan.2nd to 22nd, 2014), International Institute of Information Technology Hyderabad, and Indian Institute of Chemical Technology, Hyderabad, January 7 & 11, 2014.
- 3rd INDO-GERMAN conference on Modeling Chemical and Biochemical (Re)Activity, NIPER and IISER, Mohali, India (26th Feb. – 1st March 2013)
- Workshop on “Emerging Trends in Biomedical & Environmental Aspects with Reference to Human Health”, The National Academy of Sciences India, Allahabad (L.C.), November 07, 2012
- National Seminar on Recent Trends in Interdisciplinary Research and Astrophysics Space Science (NSRTIRASS-2012, 3-4, Nov. 2012), Department of Physics, M. B. Govt. P. G. College, Haldwani, Uttarakhand, India, November 03, 2012
- Refresher course on “Recent Trends in Chemical Sciences” (January 17 – February 05, 2012), DDU Gorakhpur University, January 21, 2012.
- “Workshop on Computer Aided Drug Design & Discovery (CAD3) - 2011” jointly organized by NIPER, Hyderabad, April 17, 2011
- “3rd International Symposium on Drug Metabolism and Pharmacokinetics (DMPK) Applications toward Drug Discovery and Development” jointly organized by Bristol –Myers Squibb, NIPER, S. A. S. Nagar (Mohali), Feb 11, 2011
- “Workshop on Experimental Tools for Characterization of Novel Materials”, organized by NCEMP and NASI The National Academic of Sciences, Allahabad, Feb. 09, 2011.
- Department of Medicinal Chemistry, NIPER, S. A. S. Nagar (Mohali), Aug. 30-Sept03, 2010.
- Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, Hyderabad, India. August 06, 2010.

- Centre for Modelling Simulation and Design, University of Hyderabad, Hyderabad, India. August 03, 2010.
- Department of Physics, DDU Gorakhpur University, Gorakhpur, India. April 12, 2006, March 4, 2008, July 2009, Feb. 2010, July 2010.
- Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, India. April 12, 2007
- Medicinal Chemistry Division, Central Drug Research Institute, Lucknow, India. March 23, 2007

AFFILIATIONS

- **Member, American Chemical Society**
- **Member, National Academic of Sciences, India, Allahabad**
- **The World Association of Theoretical and Computational Chemists (WATOC)**
- **Society of Biological Inorganic Chemistry (SBIC)**
- **Indian Biophysics Society (IBS)**

EDITOR FOR SCIENTIFIC JOURNALS:

- Editor, *Journal of Computational Biology and Bioinformatics Research*.
- Assistant editor, *Nanoscale Research Letters* (IF 2.56).
- Guest editor for special issue of *Journal of Physical Chemistry – A 112(50) (2008)* on "*Sason Shaik Festschrift*".
- Guest editor for special issue of *Journal of Physical Chemistry – A 113(43) (2009)* on "*Walter Thiel Festschrift*".

REVIEWER FOR SCIENTIFIC JOURNALS:

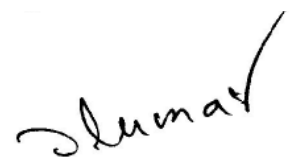
- Angewandte Chemie International Edition
- Chemical Science
- Journal of The American Chemical Society
- Journal of Computational Chemistry
- Journal of Chemical Theory and Computation
- The Journal of Physical Chemistry A
- The Journal of Physical Chemistry B
- QSAR & Combinatorial Science
- Nanoscale Research Letters
- Chemical Biology & Drug Design
- Journal of Biological Inorganic Chemistry
- Journal of Molecular Modeling
- Materials Sciences and Applications
- Chemical Physics Letters
- ChemPhysChem
- Dalton Transactions
- Journal of Organometallic Chemist

OTHERS:

- Worked as a Resource Person in “*Refresher Course on Foundations of Theoretical Methods in Physics*” organised by Department of Physics and Academic Staff College, University of Gorakhpur from Jan. 31 to Feb. 21, 1994.
- Worked as Evaluator cum Designer/ Composer in the Concurrent Evaluation of Total Literacy Campaign under National Literacy Mission (Government of India) programme in districts Azamgarh and Mau (U.P.) India
- Worked as Chief Evaluator in the Concurrent Evaluation of Total Literacy Campaign under National Literacy Mission (Government of India) programme in districts Meerut (U. P.) India.
- Organized a three days “Workshop on Computational Methods in Physical, Geological Modelling and Drug Designing” jointly organized by NCEMP, Allahabad University and NASI (Allahabad Chapter) as co-convenor.

REFERENCES:

- Prof. Dr. Walter Thiel,
Max-Planck-Institut für Kohlenforschung,
Kaiser-Wilhelm-Platz 1,
45470 Mülheim an der Ruhr, GERMANY
E-mail: thiel@mpi-muelheim.mpg.de
- Professor Sason Shaik,
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- Professor Sam P de Visser,
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Devesh Kumar

List of Publication of Dr. Devesh Kumar

A. Book Total 1
1. <i>“Iron-Containing Enzymes: Versatile Catalysts of Hydroxylation Reactions in Nature”</i> , The Royal Society of Chemistry, U.K., Eds. S. P. Visser, D. Kumar , 2011, ISBN: 978-1-84973-181-2.
B. Research Articles, Reviews & Book Chapters Total 93
95. Keto–Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. F. G. C. Reinhard, P. Barman, G. Mukherjee, J. Kumar, D. Kumar, Devesh Kumar , Chivukula V. Sastri*, and Sam P. de Visser* <i>J. Am. Chem. Soc.</i> 2017 , <i>139</i> , 18328–18338.
94. Correlation of mesogenic properties with intermolecular interaction energy for homologous series of H _n CBP. R. K. Srivastav, M. Roychoudhury, J. Kumar and Devesh Kumar *, <i>Mol Cryst. Liq. Cryst.</i> 2017 , <i>652</i> , 51 – 66.
93. A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Low-Pressure Mass Spectrometry and Computational Study. F. G. C. Reinhard, M. A. Sainna, P. Upadhyay, G. A. Balan, Devesh Kumar, S. Fornarini*, M. E. Crestoni*, and Sam P. de Visser* <i>Chem. Eur. J.</i> 2016 , <i>22</i> , 18608 – 18619.
92. Deformylation Reaction by a Nonheme Manganese(III)–PeroxoComplex via Initial Hydrogen-Atom Abstraction. P. Barman, P. Upadhyay, A. S. Faponle, J. Kumar, S. S. Nag, Devesh Kumar,* C. V. Sastri,* and S. P. de Visser* <i>Angew. Chem. Int. Ed.</i> 2016 , <i>55</i> , 11091 –11095.
91. Origin of the Enhanced Reactivity of μ -Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. M. G. Quesne, D. Senthilnathan, D. Singh, Devesh Kumar, P. Maldivi,* A. B. Sorokin,* and Sam P. de Visser,* <i>ACS Catal.</i> 2016 , <i>6</i> , 2230–2243.
90. Polarizability study of nematic liquid crystal 4-cyano-4'-pentylbiphenyl (5CB) and its nitrogen derivatives. P. Upadhyay, M. K. Rastogi, Devesh Kumar*, <i>Chem. Phys.</i> 2015 , <i>456</i> , 41-46.
89. Structure and Mechanism Leading to Formation of the Cysteine Sulfinic Acid Product Complex of a Biomimetic Cysteine Dioxygenase Model. Madleen Sallmann, Suresh Kumar, Petko Chernev, Joscha Nehrkorn, Alexander Schnegg, Devesh Kumar,* Holger Dau,* Christian Limberg,* and Sam P. de Visser*, <i>Chem. Eur. J.</i> 2015 , <i>21</i> , 7470 – 7479.
88. Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. Li Ji, A. S. Faponle, M. G. Quesne, M. A. Sainna, J. Zhang, A. Franke, Devesh Kumar, R. van Eldik, W. Liu, S. P. de Visser, <i>Chem. Eur. J.</i> 2015 , <i>21</i> , 9083 – 9092.
87. A Trimetal Carbene with Reactivity Reminiscent of Fischer–Tropsch Catalysis. M. A. Sainna, Devendra Singh, Devesh Kumar*, S. P. de Visser*, <i>Organometallics</i> 2015 , <i>34</i> , 1651-1660.
86. A comprehensive test set of epoxidation rate constants for iron(IV)–oxo porphyrin complexes. M. A. Sainna, S. Kumar, Devesh Kumar*, S. Fornarini*, M. E. Crestoni*, and S. P. de Visser*, <i>Chem.Sci.</i> 2015 , <i>6</i> , 1516–1529.
85. On copper–copper bond in hydrated cupric acetate. N. K. Shee, R. Verma, Devesh Kumar, D. Datta, <i>Computational and Theoretical Chemistry</i> 2015 , <i>1061</i> , 1-5.
84. Pyrazolo[3,4-d]pyrimidines as novel inhibitors of O-acetyl-L-serine sulfhydrylase of Entamoeba histolytica: an in silico study. U. Yadava, B. K. Shukla, M. Roychoudhury, Devesh Kumar, <i>J MolModel</i> 2015 , <i>21</i> ,96(1-13).
83. Long-Range Electron Transfer Triggers Mechanistic Differences between Iron(IV)-Oxo and Iron(IV)-Imido Oxidants. S. Kumar, A. S. Faponle, P. Barman, A. K. Vardhaman, C. V. Sastri*, Devesh Kumar*, and S. P. de Visser*, <i>J. Am. Chem. Soc.</i> 2014 , <i>136</i> , 17102-17115.
82. Properties and reactivities of nonheme iron(IV)–oxo versus iron(V)–oxo: long-range electron transfer versus hydrogen atom abstraction. B. Karamzadeh, D. Singh, W. Nam*, Devesh Kumar* and S. P. de Visser*, <i>Phys. Chem. Chem. Phys.</i> 2014 , <i>16</i> , 22611-22622.
81. A “Hemilabile” Palladium–Carbon Bond: Characterization and Its Implication in Catalysis. D. Saha, Ravi Verma, Devesh Kumar, S. Pathak, S. Bhunya, and A. Sarkar*, <i>Organometallics</i> 2014 , <i>33</i> , 3243–3246.

80. Thioether-ligated iron (II) and iron (III)-hydroperoxo/alkylperoxo complexes with an H-bond donor in the second coordination sphere. L. R. Widger, Y. Jiang, A. C. McQuilken, T. Yang, M. A. Siegler, H. Matsumura, P. Moëne-Loccoz, Devesh Kumar, S. P. de Visser*, D. P. Goldberg*, <i>Dalton Transactions</i> 2014 , 43, 7522-7532.
79. Quantum Mechanics/Molecular Mechanics Study on the Oxygen Binding and Substrate Hydroxylation Step in AlkB Repair Enzymes. M. G. Quesne, R. Latifi, L. E. Gonzalez-Ovalle, Devesh Kumar*, and S. P. de Visser*, <i>Chem. Eur. J.</i> 2014 , 20, 435 – 446.
78. Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. Anil Kumar Vardhaman, Prasenjit Barman, Suresh Kumar, C. V. Sastri,* Devesh Kumar,* and Sam P. de Visser*, <i>Chem. Commun.</i> 2013 , 49, 10926-10928.
77. Comparison of the Reactivity of Nonheme Iron(IV)–Oxo versus Iron(IV)–Imido Complexes: Which is the Better Oxidant? Anil Kumar Vardhaman, Prasenjit Barman, Suresh Kumar, C. V. Sastri,* Devesh Kumar,* and Sam P. de Visser*, <i>Angew. Chem. Int. Ed.</i> 2013 , 52,12288-12292.
76. Synthesis and Ligand Non-Innocence of Thiolate-Ligated (N ₄ S) Iron(II) and Nickel(II) Bis(imino)pyridine Complexes. L. R. Widger, Y. Jiang, M. Siegler, Devesh Kumar, R. Latifi, S. P. de Visser*, G. N. L. Jameson*and D. P. Goldberg*, <i>InorgChem</i> 2013 , 52, 10467–10480.
75. Inversion of Enantioselectivity of a Mononuclear Non-Heme Iron(II)- dependent Hydroxylase by Tuning the Interplay of Metal-Center Geometry and Protein Structure. Sarah M. Pratter, Cornelia Konstantinovics, C. L. M. DiGiuro, E. Leitner, Devesh Kumar, S. P. de Visser, G. Grogan, and G. D. Straganz*, <i>Angew. Chem. Int. Ed.</i> 2013 , 52,9677-9681.
74. Rationalization of the Barrier Height for p-Z-styrene Epoxidation by Iron(IV)-Oxo Porphyrin Cation Radicals with Variable Axial Ligands. Devesh Kumar* , Reza Latifi,* Suresh Kumar, Elena V. Rybak-Akimova, Mala A. Sainna, and Sam P. de Visser*, <i>Inorg. Chem.</i> 2013 , 52, 7968–7979.
73. Generation of a High-Valent Iron Imido Corrolazine Complex and NR Group Transfer Reactivity. Pannee Leeladee, Guy Jameson, Maxime Siegler, Devesh Kumar, Sam de Visser and David P. Goldberg, <i>Inorg. Chem.</i> 2013 , 52, 4668-4682.
72. Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes., L. E. Gonzalez-Ovalle, M. G. Quesne, Devesh Kumar* , D. P. Goldberg,* and Sam P. de Visser, <i>Org. Biomolec. Chem.</i> 2012 , 10, 5401-5409.
71. An Antimony(V) Substituted Keggin Heteropolyacid, H ₄ PSbMo ₁₁ O ₄₀ : Why is its Catalytic Activity in Oxidation Reactions so Different from that of H ₄ PVMo ₁₁ O ₄₀ ?, Hila Goldberga, Devesh Kumar ,G. Narahari Sastry,Gregory Leitus,Ronny Neumann, <i>J Mol Cat A</i> 2012 , 356, 152– 157
70. Axial Ligand Effect On The Rate Constant of Aromatic Hydroxylation By Iron(IV)- Oxo Complexes Mimicking Cytochrome P450 Enzymes, Devesh Kumar* ,G. Narahari Sastry, and Sam P. de Visser*, <i>J. Phys. Chem. B</i> 2012 , 116, 718-730
69. Mechanism of S-Oxygenation by a Cysteine Dioxygenase Model Complex, Devesh Kumar* ,G. Narahari Sastry, David P. Goldberg,* and Sam P. de Visser*, <i>J. Phys. Chem. A</i> 2012 , 116, 582-591
68. Nonheme Ferric Hydroperoxo Intermediates Are Efficient Oxidants of Bromide Oxidation, A. K. Vardhaman, C. V. Sastri*, Devesh Kumar* , and Sam P. de Visser*, <i>ChemComm</i> 2011 , 47, 11044 - 11046
67. Oxidative properties of a nonheme Ni(II)(O ₂) complex: Reactivity patterns for C–H activation, aromatic hydroxylation and heteroatom oxidation, Reza Latifi, Laleh Tahsini, Devesh Kumar* , G. Narahari Sastry, Wonwoo Nam* and Sam P. de Visser*, <i>ChemComm</i> 2011 , 47, 10674-10676.
66. Drug metabolism by Cytochrome P450: A tale of multistate reactivity, D. Kumar , “ <i>Iron-Containing Enzymes: Versatile Catalysts of Hydroxylation Reactions in Nature</i> ”, Eds. S. P. Visser, D. Kumar, The Royal Society of Chemistry, U.K., (2011) Ch. 9 pp 281-329.
65. <i>Comparison of computational methods to DNA minor groove binders</i> , Hemant Kumar Srivastava, Mukesh Chourasia, Devesh Kumar , G. N. Sastry*, <i>J. Chem. Info.Mod.</i> 2011 , 51, 558-571.

64. <i>Theoretical study on the mechanism of the oxygen activation process in cysteine dioxygenase enzymes</i> , D. Kumar* , Walter Thiel, S. P. de Visser*, J. Am. Chem. Soc. 2011 , <i>133</i> , 3869-3882.
63. <i>Effect of the Axial Ligand on Substrate Sulfoxidation Mediated by Iron (IV)–Oxo Porphyrin Cation Radical Oxidants</i> , D. Kumar* , G. N. Sastry, S. P. de Visser*, Chem. Eur. J. 2011 , <i>17</i> , 6196-6205.
62. <i>Water as biocatalyst in cytochrome P450</i> ; D. Kumar , A. Altun, S. Shaik & W. Thiel; Faraday Discussions 2011 , <i>148</i> , 373-383
61. <i>Steric Factors Override Thermodynamic Driving Force in Regioselectivity of Proline Hydroxylation by Prolyl-4-hydroxylase Enzymes</i> , Baharan Karamzadeh, D. Kumar* , G. N. Sastry, S. P. de Visser*, J. Phys. Chem. A 2010 , <i>114</i> ; 13234-13243.
60. <i>What Factors Influence the Rate Constant of Substrate Epoxidation by Compound I of Cytochrome P450 and Analogous Iron(IV)-Oxo Oxidants.</i> ; D. Kumar* , Baharan Karamzadeh, G. Narahari Sastry, S. P. de Visser*; J. Am. Chem. Soc. 2010 , <i>132</i> , 7656–7667.
59. <i>Coupling and uncoupling mechanisms in the methoxythreonine mutant of cytochrome P450cam: a quantum mechanical/ molecular mechanical study</i> ; M. Altarsha, T. Benighaus, D. Kumar & W. Thiel; J. Biol. Inorg. Chem. 2010 , <i>15</i> , 361-372.
58. <i>P450 Enzymes: Their Structure, Reactivity and Selectivity, Modeled by QM/MM Calculations</i> ; S. Shaik, S. Cohen, Y. Wang, H. Chen, D. Kumar & W. Thiel; Chem. Rev. 2010 , <i>110</i> , 949-1017.
57. <i>Effect of Porphyrin Ligands on the Regioselective Dehydrogenation versus Epoxidation of Olefins by Oxoiron(IV) Mimics of Cytochrome P450</i> ; D. Kumar* , L. Tahsini, S. P. de Visser*, H. Y. Kang, S. J. Kim, and W. Nam*; J. Phys. Chem. A 2009 , <i>113</i> , 11713-11722.
56. <i>Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: Search for an Fe(I) Oxidation State</i> ; C. S. Porro, D. Kumar & S. P. de Visser; Phys. Chem. Chem. Phys. 2009 , <i>11</i> , 10219-10226.
55. <i>A Tribute to Walter Thiel</i> ; Michael Bühl* & D. Kumar* ; J. Phys. Chem. A 2009 , <i>113</i> , 11455-11456.
54. <i>QM/MM Study of the Second Proton Transfer in the Catalytic Cycle of the D251N Mutant of Cytochrome P450cam</i> ; M. Altarsha, W. Dongqi, T. Benighaus, D. Kumar & W. Thiel; J. Phys. Chem. B 2009 , <i>113</i> , 9577-9588.
53. <i>How is the Reactivity of Cytochrome P450cam Affected by Thr252X Mutation? A QM/MM Study for X = Serine, Valine, Alanine, Glycine</i> ; M. Altarsha, T. Benighaus, D. Kumar & W. Thiel; J. Am. Chem. Soc. 2009 , <i>131</i> , 4755-4763.
52. <i>Multi-reference Ab Initio QM/MM Study on Intermediates in the Catalytic Cycle of Cytochrome P450_{cam}</i> ; A. Altun, D. Kumar , F. Neese & W. Thiel; J. Phys. Chem. A 2008 , <i>112</i> , 12904-12910.
51. <i>A Tribute to Sason Shaik</i> ; S. P.de Visser*, E. Derat* & D. Kumar* ; J. Phys. Chem. A 2008 , <i>112</i> , 12721-12723.
50. <i>A Valence Bond Modeling of Trends in Hydrogen Abstraction Barriers and Transition States of Hydrogen Reactions Catalyzed by Cytochrome P450 Enzymes</i> ; S. Shaik, D. Kumar & S. P. de Visser; J. Am. Chem. Soc. 2008 , <i>130</i> , 10128-10140.
49. <i>Theoretical Study of N-Demethylation of Substituted N,N-Dimethylanilines by Cytochrome P450: The Mechanistic Significance of Kinetic Isotope Effect Profiles</i> ; Y. Wang, D. Kumar , C. Yang, K. Han, & S. Shaik, J. Phys. Chem. B 2007 , <i>111</i> , 7700-7710.
48. <i>A Density Functional Study of the Factors that Influence the regioselectivity of Toluene Hydroxylation by Cytochrome P450 enzyme?</i> ; C. Hazan, D. Kumar , S. P. de Visser, & S. Shaik, Eur. J. Inorg. Chem. 2007 , 2966-2974.
47. <i>The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron transfer</i> ; H. Hirao, D. Kumar , H. Chen, R. Neumann, & S. Shaik, J. Phys. Chem. C 2007 , <i>111</i> , 7711-7719.

46. <i>Reactivity patterns of cytochrome P450 enzymes: Multifunctionality of the active species and the two states – two oxidants conundrum</i> , S. Shaik, H. Hirao & D. Kumar ; Natural Product Reports 2007 , <i>24</i> , 533-552.
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