

## CURRICULUM-VITAE

### Dr. DEVESH KUMAR

Associate Professor  
Department of Applied Physics  
School for Physical Sciences  
Baba Saheb Bhimrao Ambedkar University  
Vidya Vihar, Raebareli Road,  
Lucknow (U. P.) 226025 India  
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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 two different sets of experiments by two research groups on the mechanism of C-H hydroxylation by cytochrome P450 enzymes. Furthermore, the work provided answers and explanations to the nature of catalysis by cytochrome P450 enzymes
- Showed that the chemo-selectivity of a reaction can change when an electric field along one of the principle components of the system is applied. An electric field along the FeO bond preferentially leads to C-H hydroxylation, while in the opposite direction the C=C epoxidation pathway is favored
- Described the formation of CpdI ( $\text{Fe}^{\text{IV}}=\text{O}$ ) species in the non-heme system Bleomycin, which is an anti-cancerous drug

### CURRENT POSITION

Aug. 2011 – Present      Associate Professor, Department of Applied Physics,  
School for Physical Sciences, Baba Saheb Bhimrao  
Ambedkar University, Vidya Vihar, Raebareli Road,  
Lucknow (U. P.) 226025 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):

<b>Review Articles</b>	<b>Five</b>
<b>Research Papers</b>	<b>Fifty Nine</b>
<b>Editorials</b>	<b>Two</b>
<b>Book Chapter</b>	<b>Two</b>
<b>Book</b>	<b>One</b>

**Journal wise break up:**

<b>Journal</b>	<b>IF</b>	<b>No.</b>	<b>Journal</b>	<b>IF</b>	<b>No.</b>
Chem. Rev.	35.957	2	Inorg. Chem.	4.657	1
Acc. Chem. Res.	18.203	1	J. Biol. Inorg. Chem.	3.415	3
Angew. Chem. Int. Ed.	11.829	3	J. Phys. Chem. C	4.224	1
J. Am. Chem. Soc.	8.580	20	Biochemistry	3.226	1
Nat. Prod. Rep.	9.202	1	J. Chem. Info.Mod.	3.882	1
Cemm. Comm.	5.787	2	J. Inog. Biochem.	3.252	2
Chem. Eur. J.	5.382	3	J. Phys. Chem. A	2.899	6
Faraday Discuss.	3.700	1	Eur. J. Inorg. Chem.	2.941	2
Phys. Chem. Chem. Phys.	4.116	1	Other Journals	<2	12
J. Phys. Chem. B	3.471	3			

Total impact factor	:	<b>417.3</b>
Average impact factor	:	<b>6.3</b>
Citations	:	<b>1851</b>
h-index	:	<b>25</b>

## SUPERVISION EXPERIENCE

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)

## 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 Technology, 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 Technology, New Delhi* for 2010 – 2013.
3. QM/MM, MD Simulations and Computer Aided Drug Design Approaches on 5-Lipoxygenase, sponsored by *Dst-Conacyt, Mexico S&T Cooperation Programme* for 2011 – 2013.

## ADMINISTRATIVE EXPERIENCE

- |                       |   |
|-----------------------|---|
| 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

- “Workshop on Computer Aided Drug Design & Discovery (CAD3) - 2011” jointly organized by NIPER, Hyderabad, April 17, 2011
- “3<sup>rd</sup> 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

- **The World Association of Theoretical and Computational Chemists (WATOC)**
- **Society of Biological Inorganic Chemistry (SBIC) #19400**
- **Indian Biophysics Society (IBS) #L441**

## EDITOR FOR SCIENTIFIC JOURNALS:

- Editor, *Journal of Computational Biology and Bioinformatics Research*.
- Associate Editor, *International Research Journals of Biochemistry and Bioinformatics (IRJBB)*
- Assistant editor, *Nanoscale Research Letters* (IF 2.89).
- 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:

- 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

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/ Compositor 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

Devesh Kumar

## List of Publication of Dr. Devesh Kumar

<b>A. Book Total 1</b>
1. <i>"Iron-Containing Enzymes: Versatile Catalysts of Hydroxylation Reactions in Nature"</i> , The Royal Society of Chemistry, U.K., Eds. S. P. Visser, <b>D. Kumar</b> , (2012) in preparation (ISBN: 978-1-84973-181-2).
<b>B. Research Articles, Reviews &amp; Book Chapters Total 68</b>
68. Nonheme Ferric Hydroperoxo Intermediates Are Efficient Oxidants of Bromide Oxidation, A. K Vardhaman, C. V. Sastri*, <b>Devesh Kumar*</b> , and Sam P. de Visser*, <b>ChemComm 2011</b> , accepted
67. Oxidative properties of a nonheme Ni(II)(O <sub>2</sub> ) complex: Reactivity patterns for C–H activation, aromatic hydroxylation and heteroatom oxidation, Reza Latifi, Laleh Tahsini, <b>Devesh Kumar*</b> , G. Narahari Sastry, Wonwoo Nam* and Sam P. de Visser*, <b>ChemComm 2011</b> , accepted
66. Drug metabolism by Cytochrome P450: A tale of multistate reactivity, <b>D. Kumar</b> , <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., (2012) Ch. 9 pp 281-329.
65. <i>Structure and dynamics of DNA minor groove binders: A computational study</i> , Hemant Kumar Srivastava, Mukesh Chourasia, <b>Devesh Kumar</b> , G. N. Sastry*, <b>J. Chem. Info.Mod. 2011</b> , 51, 558-571.
64. <i>Quantum mechanics/molecular mechanics study on the oxygen activation process in cysteine dioxygenase enzymes</i> , <b>D. Kumar*</b> , Walter Thiel, S. P. de Visser*, <b>J. Am. Chem. Soc. 2011</b> , 133, 3869-3882.
63. <i>The axial ligand effect on substrate sulfoxidation by iron(IV)-oxo porphyrin cation radical oxidants: Predictive patterns of barrier heights and rate constants</i> , <b>D. Kumar*</b> , G. N. Sastry, S. P. de Visser*, <b>Chem. Eur. J. 2011</b> , 17, 6196-6205.
62. <i>Water as biocatalyst in cytochrome P450</i> ; <b>D. Kumar</b> , A. Altun, S. Shaik & W. Thiel; <b>Faraday Discussions 2011</b> , 148, 373-383
61. <i>Steric Factors Override Thermodynamic Driving Force in Regioselectivity of Proline Hydroxylation by Prolyl-4-hydroxylase Enzymes</i> , Baharan Karamzadeh, <b>D. Kumar*</b> , G. N. Sastry, S. P. de Visser*, <b>J. Phys. Chem. A 2010</b> , 114; 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> ; <b>D. Kumar*</b> , Baharan Karamzadeh, G. Narahari Sastry, S. P. de Visser*; <b>J. Am. Chem. Soc. 2010</b> , 132, 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, <b>D. Kumar</b> & W. Thiel; <b>J. Biol. Inorg. Chem. 2010</b> , 15, 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, <b>D. Kumar</b> & W. Thiel; <b>Chem. Rev. 2010</b> , 110, 949-1017.
57. <i>Effect of Porphyrin Ligands on the Regioselective Dehydrogenation versus Epoxidation of Olefins by Oxoiron(IV) Mimics of Cytochrome P450</i> ; <b>D. Kumar*</b> , L. Tahsini, S. P. de Visser*, H. Y. Kang, S. J. Kim,   and W. Nam*; <b>J. Phys. Chem. A 2009</b> , 113, 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, <b>D. Kumar</b> & S. P. de Visser; <b>Phys. Chem. Chem. Phys. 2009</b> , 11, 10219-10226.
55. <i>A Tribute to Walter Thiel</i> ; Michael Bühl* & <b>D. Kumar*</b> ; <b>J. Phys. Chem. A 2009</b> , 113, 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, <b>D. Kumar</b> & W. Thiel; <b>J. Phys. Chem. B 2009</b> , 113, 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, <b>D. Kumar</b> & W. Thiel; <b>J. Am. Chem. Soc.</b> <b>2009</b> , <i>131</i> , 4755-4763.
52. <i>Multi-reference Ab Initio QM/MM Study on Intermediates in the Catalytic Cycle of Cytochrome P450<sub>cam</sub></i> ; A. Altun, <b>D. Kumar</b> , F. Neese & W. Thiel; <b>J. Phys. Chem. A</b> <b>2008</b> , <i>112</i> , 12904-12910.
51. <i>A Tribute to Sason Shaik</i> ; S. P. de Visser*, E. Derat* & <b>D. Kumar*</b> ; <b>J. Phys. Chem. A</b> <b>2008</b> , <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, <b>D. Kumar</b> & S. P. de Visser; <b>J. Am. Chem. Soc.</b> <b>2008</b> , <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, <b>D. Kumar</b> , C. Yang, K. Han, & S. Shaik, <b>J. Phys. Chem. B</b> <b>2007</b> , <i>111</i> , 7700-7710.
48. <i>A Density Functional Study into the Factors that Influence the Chemoselectivity of Toluene Hydroxylation by Cytochrome P450 enzyme?</i> ; C. Hazan, <b>D. Kumar</b> , S. P. de Visser, & S. Shaik, <b>Eur. J. Inorg. Chem.</b> <b>2007</b> , 2966-2974.
47. <i>The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron</i> ; H. Hirao, <b>D. Kumar</b> , H. Chen, R. Neumann, & S. Shaik, <b>J. Phys. Chem. C</b> <b>2007</b> , <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 & <b>D. Kumar</b> ; <b>Natural Product Reports</b> <b>2007</b> , <i>24</i> , 533-552.
45. <i>Reactivity of High-Valent Iron Oxo Species in Enzymes and Synthetic Reagents: A Tale of Many States</i> ; S. Shaik, H. Hirao & <b>D. Kumar</b> , <b>Acc. Chem. Res.</b> <b>2007</b> , <i>40</i> , 532-542.
44. <i>Singlet Diradical Character of an Oxidized Ruthenium Trithiolate: Electronic Structure and Reactivity</i> ; C. A. Grapperhaus, P. M. Kozlowski, <b>D. Kumar</b> , H. N. Frye, K. B. Venna, & S. Poturovic, <b>Angew. Chem. Int. Ed.</b> <b>2007</b> , <i>119</i> , 1-5.
43. <i>Formation of the Active Species of Cytochrome P450 Using Iodosylbenzene: A Case for Spin Selective Reactivity</i> ; K.-B. Cho, Y. Moreau, <b>D. Kumar</b> , D. Rock, J. P. Jones & S. Shaik, <b>Chem. Eur. J.</b> <b>2007</b> , <i>13</i> , 4103 - 4115.
42. <i>On the Identity and Reactivity Patterns of the "Second Oxidant" of the T252A Mutant of Cytochrome P450cam in the Oxidation of 5-Methylenenylcamphor</i> ; H. Hirao, <b>D. Kumar</b> & S. Shaik, <b>J. Ing. Biochem.</b> <b>2006</b> , <i>100</i> , 2054-2068.
41. <i>Bleomycin: A Poulos-Kraut Mechanism of O-O Activation for the Formation of a Compound I Type Species</i> ; D. Kumar, H. Hirao, S. Shaik & P. M. Kozlowski, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 16148-16158.
40. <i>Characterization of Manganese(V) Oxo Polyoxometalate Intermediates and their Properties in Oxygen Transfer Reactions</i> ; A. M. Khenkin, <b>D. Kumar</b> , S. Shaik & R. Neumann, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 15451-15460.
39. <i>Seeking for New Catalysts for Monooxygenations Made from Polyoxometalate: An Iron-Oxo derivative of the Lindqvist Anion</i> ; E. Derat, <b>D. Kumar</b> , R. Neumann & S. Shaik, <b>Inorg. Chem.</b> <b>2006</b> , <i>45</i> , 8655-8663.
38. <i>Ferromagnetic Bonding: High Spin Copper Clusters (<sup>n+1</sup>Cu<sub>n</sub>; n = 2-12) Devoid of Electron Pairs But Possessing Strong Bonding</i> ; S. P. de Visser, <b>D. Kumar</b> , M. Danovich, N. Nevo, D. Danovich, P. K. Sharma, W. Wu & S. Shaik, <b>J. Phys. Chem. A</b> <b>2006</b> , <i>110</i> , 8510-8518.

37. <i>Two-State Reactivity in Alkane Hydroxylation by Non-Heme Iron-Oxo Complexes</i> ; H. Hirao, <b>D. Kumar</b> , Lawrence Que Jr. & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 8590-8606.
36. <i>In silico design of a mutant of cytochrome P450 containing selenocysteine</i> ; S. Cohen, <b>D. Kumar</b> & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 2649-2653.
35. <i>Gauging the Relative Oxidative Powers of Compound I, Ferric-Hydroperoxide and the Ferric-Hydrogen Peroxide Species of Cytochrome P450 Towards C-H Hydroxylation of a Radical Probe Substrate</i> ; E. Derat, <b>D. Kumar</b> , H. Hirao, & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 473-484.
34. <i>Kinetic Isotope Effect is A Sensitive Probe of Spin State Reactivity in C-H Hydroxylation of N,N-Dimethyl Aniline by Cytochrome P450</i> ; C. Li, W. Wu, <b>D. Kumar</b> , & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2006</b> , <i>128</i> , 394-395.
33. <i>The High-Valent Iron-Oxo Species of Polyoxometalate, If can be Made, Will be a Highly Potent Catalyst for C-H Hydroxylation and Double Bond Epoxidation</i> ; <b>D. Kumar</b> , E. Derat, A. M. Khenkin, R. Neumann & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2005</b> , <i>127</i> , 17712-17718.
32. <i>New Feature in the Catalytic Cycle of Cytochrome P450: A "Surprise" Intermediate en-Route to Compound I?</i> ; <b>D. Kumar</b> , H. Hirao, S. P. de Visser, J. Zheng, D. Wang, W. Thiel & S. Shaik, <b>J. Phys. Chem. B</b> <b>2005</b> , <i>109</i> , 19946-19951.
31. <i>Two States and Two More in the Mechanisms of Hydroxylation and Epoxidation by Cytochrome P450</i> ; H. Hirao, <b>D. Kumar</b> , W. Thiel & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2005</b> , <i>127</i> , 13007-13018.
30. <i>A Theoretical Perspective on Structure and Mechanisms of Cytochrome P450 Enzymes</i> ; S. Shaik, <b>D. Kumar</b> , S. P. de Visser, A. Ahmet & W. Thiel, <b>Chem. Rev.</b> <b>2005</b> , <i>105</i> , 2279-2328. Recognized as a <b>Hot Paper</b> by <b>Thomson ISI's Essential Science Indicators</b> Nov. 2006 .
29. <i>Sulfoxidation Mechanisms Catalyzed by Cytochrome P450 and Horseradish Peroxidase Models: Spin-Selection Induced by the Ligand</i> ; <b>D. Kumar</b> , S. P. de Visser, P. K. Sharma, H. Hirao & S. Shaik, <b>Biochemistry</b> <b>2005</b> , <i>44</i> , 8148-8158.
28. <i>Theory Favors A Stepwise Mechanism of Porphyrin Degradation By a Ferric Hydroperoxide Model of Active Speices of Heme Oxygenase</i> ; <b>D. Kumar</b> , S. P. de Visser, & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2005</b> , <i>127</i> , 8204-8213.
27. <i>Theoretical Investigation of C-H Hydroxylation by (N4Py)Fe<sup>IV</sup>=O<sup>2+</sup>: An Oxidant More Powerful than P450?</i> ; <b>D. Kumar</b> , H. Hirao, Lawrence Que Jr. & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2005</b> , <i>127</i> , 8026 -8027.
26. <i>The Intrinsic Axial Ligand Effect on Propene Oxidation by Horseradish Peroxidase versus Cytochrome P450 Enzymes</i> ; <b>D. Kumar</b> , S. P. de Visser, P. K. Sharma, E. Derat & S. Shaik, <b>J. Biol. Inorg. Chem.</b> <b>2005</b> , <i>10</i> , 181-189.
25. <i>Multi-state Reactivity in Styrene Epoxidation by Compound I of Cytochrome P450: Mechanisms of Products and Side Product Formations</i> ; <b>D. Kumar</b> , S. P. de Visser & S. Shaik, <b>Chem. Eur. J.</b> <b>2005</b> , <i>11</i> , 2825-2835.
24. <i>Computer Generated High Valent Iron-Oxo and Manganese-Oxo Species with Polyoxometalate Ligands-How do they Compare with the Iron-Oxo Active Species of Heme Enzymes?</i> S. P. de Visser, <b>D. Kumar</b> , R. Neumann & S. Shaik, <b>Angw. Chem. Int. Ed.</b> <b>2004</b> , <i>43</i> , 5661-5665.
23. <i>One oxidant, many pathways: A theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes</i> ; S. Shaik, S. P. de Visser, D. Kumar, <b>J. Biol. Inorg. Chem.</b> <b>2004</b> , <i>9</i> , 661-668.
22. <i>An External Electric Field Will Control the Selectivity of Enzyme-Like Bond Activations</i> ; S. Shaik, S. P. de Visser & <b>D. Kumar</b> , <b>J. Am. Chem. Soc.</b> <b>2004</b> , <i>126</i> , 11746-11749.
21. <i>A Predictive Pattern of Computed Barriers for C-H Hydroxylation by Compound I of Cytochrome P450</i> ; S. P. de Visser, <b>D. Kumar</b> , S. Cohen, R. Shacham & S. Shaik, <b>J. Am. Chem. Soc.</b> <b>2004</b> , <i>126</i> , 8362-8363.



20. The "Rebound Controversy": An Overview and Theoretical Modeling of the Rebound Step in C-H Hydroxylation by Cytochrome P450; S. Shaik, S. Cohen, S. P. de Visser, P. K. Sharma, <b>D. Kumar</b> , S. Kozuch, F. Ogliaro & D. Danovich, <i>Eur. J. Inorg. Chem.</i> <b>2004</b> , 207-226.
19. How Do Aldehyde Side Products Occur During Alkene Epoxidation by Cytochrome P450? Theory Reveals a State-Specific Multi-State Scenario Where the High-Spin Component Leads to All Side Products; S. P. de Visser, <b>D. Kumar</b> , & S. Shaik, <i>J. Inorg. Biochem.</i> <b>2004</b> , 98, 1183-1193.
18. Oxygen Economy of Cytochrome P450: What is the Origin of the Mixed Functionality as a Dehydrogenating-Oxidase Enzyme Compared with its Normal Function?; <b>D. Kumar</b> , S. P. de Visser, & S. Shaik, <i>J. Am. Chem. Soc.</i> <b>2004</b> , 126, 5072-5073.
17. Porphyrin Traps its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450; P. K. Sharma, R. Kerkokiants, S. P. de Visser, <b>D. Kumar</b> & S. Shaik, <i>Angew. Chem. Int. Ed.</i> <b>2004</b> , 43, 1129-1132.
16. Radical Clock Substrates, their C-H Hydroxylation Mechanism by Cytochrome P450 and Other Reactivity Patterns; What Does Theory Reveal About the Clocks'- Behavior?; <b>D. Kumar</b> , S. P. de Visser, P. K. Sharma, S. Cohen & S. Shaik, <i>J. Am. Chem. Soc.</i> <b>2004</b> , 126, 1907-1920.
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