Full List of Peer Reviewed Publications:

Journal Articles:

1. Vaishali Thakkur, Chandan Kumar Das, Shivani Verma, Suman Saha, Nisanth N. Nair
Methyl substituted β-lactam framework based antibiotics and β-lactamase inhibitors: Proof of concept by computations, bioRxiv (2024). (DOI: 10.1101/2024.01.14.575563)

2. Ritama Kar, Sagarmoy Mandal, Vaishali Thakkur, Bernd Meyer, Nisanth N. Nair
Speeding-up Hybrid Functional-Based Ab Initio Molecular Dynamics Using Multiple Time-stepping and Resonance-Free Thermostat, J. Chem. Theory Comput. **19** 8351 (2023). (DOI: 10.1039/d3cp00521f)

3. Chandan Kumar Das, Abhinav Gupta, Nisanth N. Nair
Probing the general base for DNA polymerization in telomerase: a molecular dynamics investigation, Phys Chem Chem Phys **25**, 14147 (2023). (DOI: 10.1039/d3cp00521f)

4. Shubhendra Tripathi, Nisanth N. Nair
Temperature Accelerated Sliced Sampling to Probe Ligand Dissociation from Protein, J. Chem. Inf. Model **63**, 5182 (2023) (DOI: 10.1021/acs.jcim.3c00376)

5. Shitanshu Bajpai, Brian Petkov, Muchen Tong, Charlles Abreu, Nisanth N. Nair, Mark Tuckerman
An interoperable implementation of collective-variable based enhanced sampling methods in extended phase space within the OpenMM package, J. Comput. Chem. **44**, 2166 (2023). (DOI: https://doi.org/10.1002/jcc.27182 & 10.26434/chemrxiv-2023-wwxq2)

6. Shivani Verma; Nisanth N. Nair
Computational Study of pKa Shift of Aspartate Residue in Thioredoxin: Role of Conformational Sampling J. Chem. Sci., **135**, 75 (2023). (arXiv:2211.13637v1)

7. Sagarmoy Mandal, Ritama Kar, Bernd Meyer, Nisanth N. Nair
Hybrid Functional and Plane Waves based Ab Initio Molecular Dynamics Study of the Aqueous Fe2+/Fe3+ Redox Reaction, ChemPhysChem, **24**, e202200617 (2023); DOI: 10.1002/cphc.202200617

8. Rahul Verma; Nisanth N. Nair
Proton-Exchange Reaction in Acidic Zeolites: Mechanism and Free Energetics, J. Phys. Chem. C, **126**, 19169–19177 (2022); DOI: 10.1021/acs.jpcc.2c06146.

9. Vaishali Thakkur, Chandan Kumar Das, Nisanth N. Nair
Inhibition Mechanism of Class D β-Lactamases by Avibactam, ACS Catal. **12**, 10338−10352 (2022); DOI: 10.1021/acscatal.2c02693.

10. Abhinav Gupta, Shivani Verma, Ramsha Javed, Suraj Sudhakar, Saurabh Srivastava, Nisanth N. Nair
Exploration of high dimensional free energy landscapes by a combination of temperature-accelerated sliced sampling and parallel biasing, J. Comput. Chem. **43**, 1186-1200 (2022); DOI: 10.1002/jcc.26882.

11. Sagarmoy Mandal, Ritama Kar, Tobias Klöffel, Bernd Meyer, Nisanth N. Nair
Improving the scaling and performance of multiple time stepping-based molecular dynamics with hybrid density functionals, J. Comput. Chem. **43**, 588-597 (2022); (DOI: 10.1002/jcc.26816).

12. Anji Babu Kapakayala, Nisanth N. Nair
Boosting the Conformational Sampling by Combining Replica Exchange with Solute Tempering and Well-Sliced Metadynamics, J. Comput. Chem. **42**, 2233-2240 (2021); (DOI:10.1002/jcc.26752 & **arXiv:2108.13641**).

13. Asit Pal, Subhendu Pal, Shivani Verma, Motoyuki Shiga, Nisanth N. Nair
Mean Force Based Temperature Accelerated Sliced Sampling: Efficient Reconstruction of High Dimensional Free Energy Landscapes, J. Comput. Chem. **42**, 1996-2003 (2021); (DOI: 10.1002/jcc.26727)

14. S. Mandal, V. Thakkur, Nisanth N. Nair, *Achieving an Order of Magnitude Speedup in Hybrid-Functional- and Plane-Wave-Based Ab Initio Molecular Dynamics: Applications to Proton-Transfer Reactions in Enzymes and in Solution*, J. Chem. Theory Comput. **17**, 2244 (2021). (DOI: 10.1021/acs.jctc.1c00009)

15. Neha Vithani, Balaji Prakash, Nisanth N Nair, *Mechanism of Nucleotidyltransfer Reaction and Role of Mg2+ Ion in Sugar Nucleotidyltransferases*, Biophys. J. **119**, 619-627 (2020).

16. C. K. Das, Nisanth N. Nair *Elucidating the Molecular Basis of Avibactam Mediated Inhibition of Class A β-Lactamases*, Chem. Eur. J. **26**, 9639-9651 (2020).

17. S. Mandal, Nisanth N. Nair, *Efficient computation of free energy surfaces of chemical reactions using ab initio molecular dynamics with hybrid functionals and plane waves* , J. Comput. Chem. **41**, 1790 (2020).

18. Irfan Qayoom, Rahul Verma, Prem Anand Murugan, Deepak Bushan Raina, Arun Kumar Teotia, Saravanan Matheshwaran, Nisanth N. Nair, Magnus Taegil, Lars Lidgren, Ashok Kumar, *A biphasic nanohydroxyapatite/calcium sulphate carrier containing Rifampicin and Isoniazid for local delivery gives sustained and effective antibiotic release and prevents biofilm formation* , Scientific Reports **10**, 14128, (2020).

19. S. Mandal, Nisanth N. Nair, *Speeding-up ab initio molecular dynamics with hybrid functionals using adaptively compressed exchange operator based multiple timestepping*, J. Chem. Phys. [Letter*]* **151**, 151102 (2019).

20. S. Paul, Nisanth N. Nair, H. Vashisth, *Phase space and collective variable based simulation methods for studies of rare events* , Mol. Sim. **45**, 1273-1284 (2019).

21. A. B. Kapakayala, A. Gupta, S. Verma, Nisanth N. Nair, *Free energy calculations of alanine tripeptide in explicit water using temperature accelerated sliced sampling* , J. Ind. Chem. Soc. **96**, 875-882 (2019).

22. S. Kunnikuruvan, Nisanth N. Nair, *Mechanistic Insights into the Brønsted Acid-Catalyzed Dehydration of β-d-Glucose to 5-Hydroxymethylfurfural under Ambient and Subcritical Conditions* ACS Catal. **9**, 7250-7263 (2019); *ACS Catal.* **9**, 8452-8452 (2019).

23. K. Soniya, S. Awasthi, Nisanth N. Nair, Amalendu Chandra, *Transimination Reaction at the Active Site of Aspartate Aminotransferase: A Proton Hopping Mechanism through Pyridoxal 5'-Phosphate* , *ACS Catal.* **9**, 6726-6283 (2019).

24. S. Awasthi, Nisanth N. Nair, *Exploring high-dimensional free energy landscapes of chemical reactions* , *Wiley Interdisciplinary Reviews: Comput. Mol. Sci.* **9**, e1398 (2019).

25. A. Panjla, G. Kaul, M. Shukla, S. Tripathi, Nisanth N. Nair, S. Chopra, Sandeep Verma, *A novel molecular scaffold resensitizes multidrug-resistant S. aureus to fluoroquinolones* , *Chem. Comm.* **55**, 8599-8602 (2019).

26. S. Mandal, J. Debnath, B. Meyer, Nisanth N. Nair *Enhanced sampling and free energy calculations with hybrid functionals and plane waves for chemical reactions J. Chem. Phys. **149**, 144113 (2018).*

27. Sudhir K Sahoo and Nisanth N. Nair *Interfacing the Core-Shell or the Drude Polarizable Force Field With Car–Parrinello Molecular Dynamics for QM/MM Simulations* *Frontiers in Chemistry* ***6****, 275 (2018).*

28. Shalini Awasthi, Shalini Gupta, Ravi Tripathi and Nisanth N Nair *Mechanism and Kinetics of Aztreonam Hydrolysis Catalyzed by Class-C β-Lactamase: A Temperature-Accelerated Sliced Sampling Study* J. Phys. Chem. B. **122**, 4299-4308 (2018).

29. Chandan K. Das and Nisanth N. Nair *Molecular insights into avibactam mediated class C β-lactamase inhibition: competition between reverse acylation and hydrolysis through desulfation* Phys. Chem. Chem. Phys. **20**, 14482-14490 (2018).

30. Neha Vithani, Pravin Kumar, Ankush Jagtap, Sunil Kumar Verma, Ravi Tripathi, Shalini Awasthi, Nisanth N.Nair, Balaji Prakash *Mechanism of Mg^{2+}-Accompanied Product Release in Sugar Nucleotidyltransferases* Structure **26,** 459-466 (2018).

31. A Kumar, V Sudarkodi, Priya V Parandekar, Nishant K Sinha, Om Prakash, Nisanth N Nair, Sumit Basu *Adhesion between a rutile surface and a polyimide: a coarse grained molecular dynamics study* Model. Sim. Mat. Sci. Eng. **26,** 035012 (2018).

32. V Sudarkodi, K Sooraj, Nisanth N. Nair, Sumit Basu, Priya V Parandekar, Nishant K Sinha, Om Prakash and Tom Tsotsis *Mechanical response of two polyimides through coarse-grained molecular dynamics simulations* *Model. Sim. Mat. Sci. Eng.* **26,** 025013 (2018).

33. Jayashrita Debnath, Sooraj Kunnikuruvan, Nishant Sinha, Priya V Parandekar, Om Prakash, Thomas K Tsotsis, Nisanth N. Nair *A database-based approach for predicting coupled cascade reaction kinetics in polymers: application to oxidative degradation kinetics of high-performance polymers* Molecular Simulation **44,** 582-589 (2018).

34. Kalpana Tomar, Satyendra Soni, Pratibha Bhadauriya, Rashmi Parihar, Subramaniam Ganesh, Nisanth N. Nair, Gurunath Ramanathan *Mercuric Ion Sensing by an Overlapping β -turn Containing Peptide* Chemistry Select **2,** 8072-8075 (2017).

35. Sooraj Kunnikuruvan, Priya V Parandekar, Om Prakash, Thomas K Tsotsis, and Nisanth N Nair *Polymerization mechanism and cross-link structure of nadic end-capped polymers: a quantum mechanical and microkinetic investigation* Macromolecules **50**, 6081-6087 (2017).

36. Giuseppe Fisicaro, Luigi Genovese, Oliviero Andreussi, Sagarmoy Mandal, Nisanth N. Nair, Nicola Marzari, and Stefan Goedecker *Soft-sphere continuum solvation in electronic-structure calculations* J. Chem. Theor. Comput. **13,** 3829–3845 (2017).

37. Shalini Awasthi and Nisanth N. Nair *Exploring high dimensional free energy landscapes: Temperature accelerated sliced sampling '* J. Chem. Phys. **146,** 094108 (2017).

38. Chandan K Das and Nisanth N. Nair *Hydrolysis of Cephalexin and Meropenem by New Delhi Metallo β-Lactamase: Substrate Protonation Mechanism is Drug Dependent Phys.* Chem. Chem. Phys. **19**, 13111-13121 (2017).

39. N. Vithani, S. Batra, B. Prakash, Nisanth N. Nair *Elucidating the GTP Hydrolysis Mechanism in FeoB, a Hydrophobic Amino Acid Substituted GTPase* ACS Catal. (Letter) **7** 902-906 (2017).

40. Venkataramana Imandi and Nisanth N. Nair *The Wacker Oxidation of Allyl Alcohol along Cyclic-Intermediate Routes: an Ab Initio Molecular Dynamics Investigation* Chemical Physics Letters **660,** 111-116 (2016).

41. Sooraj Kunnikuruvan, Priya V. Parandekar, Om Prakash, Tom K. Tsotsis, and Nisanth N. Nair *Insights into the Mechanism and Kinetics of Thermo-Oxidative Degradation of HFPE High Performance Polymerç* J. Phys. Chem. B. **120,** 4852-4860 (2016).

42. Sudhir K. Sahoo and Nisanth N. Nair *CPMD/GULP QM/MM Interface for Modeling Periodic Solids: Implementation and its Application in the Study of Y-Zeolite Supported Rhn Clusters* J. Comput. Chem. **37,** 1657-1667 (2016).

43. Ravi Tripathi, and Nisanth N. Nair *Deacylation Mechanism and Kinetics of Acyl-Enzyme Complex of Class-C β-Lactamase and Cephalothin* J. Phys. Chem. B **120,** 2681-2690 (2016).

44. Shalini Awasthi, Venkat Kapil and Nisanth N. Nair *Sampling Free Energy Surfaces as Slices by Combining Umbrella Sampling and Metadynamics* J. Comput. Chem. **37,** 1413-1424 (2016).

45. Sudhir K. Sahoo and Nisanth N. Nair *A Potential with Low Point Charges for Pure Siliceous Zeolites* J. Comput. Chem. **36,** 1562-1567 (2015).

46. Venkataramana Imandi and Nisanth N. Nair *Can the Absence of Isotope Scrambling in the Wacker Oxidation of Allyl Alcohol Disprove Outer Sphere Hydroxypalladation?* J. Phys. Chem. B. **36,** 1562-1567 (2015).

47. Sooraj Kunnikuruvan, Priya V. Parandekar, Om Prakash, Tom K. Tsotsis, Sumit Basu and Nisanth N. Nair *Quantum Mechanical Computations and Microkinetic Modeling to Obtain Mechanism and Kinetics of Oxidative Degradation of a Polyimide* Macromol. Theory and Sim. **24,** 344-351 (2015).

48. Ravi Tripathi and Nisanth N. Nair *Mechanism of Meropenem Hydrolysis by New Delhi Metallo β-Lactamase* ACS Catalysis **5,** 2577-2586 (2015).

49. N. Sadanandam, Nisanth N. Nair and J. K. Singh *Interaction Potential Models for Bulk ZnS, ZnS Nanoparticle, and ZnS Nanoparticle-PMMA From First-Principles* J. Comput. Chem. **36,** 1176-1186 (2015).

50. Tushar K. Ghosh and Nisanth N. Nair *Nature of β-TaON Surfaces at Ambient Conditions* Surf. Sci. **635**, 19-26 (2015).

51. Tushar K. Ghosh and Nisanth N. Nair *Alumina-Supported Rh, Rh2, and RhI(CO) as Catalysts for Hydrogen Evolution from Water* Surf. Sci. **632**, 20-27 (2015).

52. Md. E. Ali, N. N. Nair, M. Retegan, F. Neese, V. Staemmler, D. Marx *The iron-sulfur core in Rieske proteins is not symmetric* J. Biol. Inorg. Chem. **19**, 1287-1293 (2014).

53. András Stirling, Nisanth N. Nair, Agustí Lledós and Gregori Ujaque, *Challenges in modelling homogenous catalysis: new answers from ab initio molecular dynamics to the controversy over the Wacker Process ,* Chem. Soc. Rev. **43**, 4940-4952 (2014).

54. Ambar Banerjee, Gaurab Ganguly, Ravi Tripathi, Nisanth N. Nair and Ankan Paul *Unearthing the mechanism of prebiotic nitrile bond reduction in hydrogen cyanide through a curious association of two molecular radical anions* Chem. Eur. J **20**, 6348-6357 (2014).

55. Sudharsan Pandiyan, Priya V. Parandekar, Om Prakash, Thomas K. Tsotsis, Nisanth N. Nair, Sumit Basu *Controlling the sub-molecular motions to increase the glass transition temperature of polymers* Chem. Phys. Lett. **593**, 24-27 (2014).

56. Ravi Tripathi, and Nisanth N. Nair *Mechanism of Acyl-Enzyme Complex Formation from the Henry-Michaelis Complex of Class C β-Lactamase with β-Lactam Antibiotics* J. Am. Chem. Soc. **135**,14679-14690 (2013).

57. Sourav Bhunya, Ambar Banerjee, Ravi Tripathi, Nisanth N. Nair, and Ankan Paul *Ammonia-Borane Dehydrogenation Via an Unexpected Pentacoordinate Boron Species: Insights from density Functional and Molecular Dynamics studies* Chem. Eur. J. **19**, 17673-17678 (2013).

58. Johannes Frenzel, Janos Kiss, Nisanth N. Nair, Bernd Meyer, and Dominik Marx *Methanol synthesis on ZnO from molecular dynamics* Physica Status Solidi (B) **250**,1174-1190 (2013).

59. Venkataramana Imandi, Sooraj K., and Nisanth N. Nair *Hydroxypalladation Precedes Rate Determining Step in the Wacker Oxidation of Ethene* Chem. Eur. J. **19**,4724-4731 (2013). [Highlighted as Very Important Paper]

60. Tushar K. Ghosh, and Nisanth N. Nair *Rh1/ γ-Al2O3 Single Atom Catalysis of O2 Activation and CO Oxidation: Mechanism, Effects of Hydration, Oxidation State and Cluster Size* ChemCatChem **5**, 1811-1821 (2013).

61. Susan Sen, Nisanth N. Nair, Teppei Yamada, Hiroshi Kitagawa, and Parimal K. Bharadwaj *High Proton Conductivity by a Metal-Organic Framework Incorporating Zn8O Clusters with Aligned Imidazolium Groups Decorating the Channels* J. Am. Chem. Soc. **134**, 19432-19437 (2012).

62. Sooraj K., S. Batra and Nisanth N. Nair *Enhancing the Reaction Rates of Morita-Baylis-Hillman Reaction in Heterocyclic Aldehydes by Substitutions* Chem. Phys. Chem. **13**, 3723-3730 (2012).

63. Md. Ehesan Ali, Nisanth N. Nair, V. Staemmler and D. Marx *Constrained spin-density dynamics of an iron-sulfur complex: Ferredoxin cofactor* J. Chem. Phys. **136**, 224101 (2012).

64. Ravi Tripathi and Nisanth N. Nair *Thermodynamic and Kinetic Stabilities of Active Site Protonation States of Class C β-Lactamase* J. Phys. Chem. B **116**, 4741-4753 (2012).

65. Basanta K. Rajbongshi, Nisanth N. Nair, M. Nethaji, and Gurunath Ramanathan *Segregation into Chiral Enantiomeric Conformations of an Achiral Molecule by Concomitant Polymorphism* Crystal Growth and Design **12**, 1823-1829 (2012).

66. Jarugu Narasimha Moorthy, Kalyan Senapati, Keshaba Nanda Parida, Samik Jhulki, Kunnikuruvan Sooraj, and Nisanth N. Nair *Twist Does a Twist to the Reactivity: Stoichiometric and Catalytic Oxidations with Twisted Tetramethyl-IBX*
J. Org. Chem. **76**, 9593-9601 (2011).

67. Shahnawaz Rafiq, Basanta Kumar Rajbongshi, Nisanth N. Nair, Pratik Sen, and Gurunath Ramanathan. *Excited State Relaxation Dynamics of Model Green Fluorescent Protein Chromophore Analogs: Evidence for cis-trans isomerism*
J. Phys. Chem. A. **115**, 13733-13742 (2011).

68. Tushar K. Ghosh and Nisanth N. Nair *Oxidative Addition of Water to Rhn (n=1-4) Clusters on Alumina Surfaces and Spontaneous Formation of H2* J. Phys. Chem. C. **115**, 15403-15409 (2011)

69. Nisanth N. Nair *Ligand Exchanges and Hydroxypalladation Reactions of the Wacker Process in Aqueous Solution at High Cl- Concentration ,* J. Phys. Chem. B. **115**, 2312-2321 (2011).

70. V. Chandrasekhar, B. Mahanti, P. Bandipalli, K. Bhanuprakash, Nisanth N. Nair. *Cyclometalated Ir(III) complexes containing N-aryl picolinamide ancillary ligands* J. Organometallic Chem. **696**, 2711-2719 (2011).

71. E. Schreiner, Nisanth N. Nair, C. Wittekindt, D. Marx. *Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions and Pyrite Mineral Surfaces on Formation and Hydrolysis of Peptides* J. Am. Chem. Soc. **133**, 8216-8226 (2011).

72. R. Pollet, Nisanth N. Nair, D. Marx. *The water exchange of ProHance MRI contrast agent: Isomer-dependent free energy landscapes and mechanisms* Inorg. Chem. **50**, 4791-4797 (2011).

73. Harald Forbert, Marco Masia, Anna Kaczmarek-Kedziera, Nisanth N. Nair, and Dominik Marx. *Aggregation-Induced Chemical Reactions: Acid Dissociation in Growing Water Clusters* J. Am. Chem. Soc. **133**, 4062-4072 (2011).

74. Janos Kiss, Johannes Frenzel, Nisanth N. Nair, Bernd Meyer, and Dominik Marx. *Methanol synthesis on ZnO(000). III. Free energy landscapes, reaction pathways, and mechanistic insights* J. Chem. Phys. **134**, 064710 (2011).

75. P. M. Kowalski, M. Farnesi Camellone, N. N. Nair, B. Meyer, D. Marx. *Charge Localization Dynamics induced by Oxygen Vacancies on the Titania TiO2(110) Surface ,* Phys. Rev. Lett. **105**, 146405 (2010)

76. S. Annamaria Fiethen, V. Staemmler, N. N. Nair, J. Ribas-Arino, E. Schreiner, D. Marx. *Revealing the Magnetostructural Dynamics of [2Fe-2S] Ferredoxins from Reduced-Dimensionality Analysis of Antiferromagnetic Exchange Coupling Fluctuations* J. Phys. Chem. B **114**, 11612-11619 (2010)

77. N. N. Nair, J. Ribas-Arino, V. Staemmler, D. Marx. *Magnetostructural Dynamics from Hubbard-U Corrected Spin-Projection [2Fe-2S] Complex in Ferredoxin* J. Chem. Theor. Comput. **6**, 569-575 (2010)

78. E. Schreiner, N. N. Nair, D. Marx. *Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions on Peptide Bond Formation and Peptide Hydrolysis* J. Am. Chem. Soc. **131**, 13668-13675 (2009)

79. N. N. Nair, E. Schreiner, D. Marx, *Peptide Synthesis in Aqueous Environments: The Role of Extreme Conditions on Amino Acid Activation* J. Am. Chem. Soc. **130**, 14148-14160 (2008)

80. N. N. Nair, E. Schreiner, R. Pollet, V. Staemmler, D. Marx, *Magnetostructural Dynamics with the Extended Broken Symmetry Formalism: Antiferromagnetic [2Fe–2S] Complexes* J. Chem. Theory Comput. **4**, 1174-1188 (2008)

81. E. Schreiner, N. N. Nair, D. Marx, *Influence of Extreme Thermodynamic Conditions and Pyrite Surfaces on Peptide Synthesis in Aqueous Media* J. Am. Chem. Soc. **130**, 2768-2770 (2008) (Three–Page Communication to the Editor)

82. N. N. Nair, E. Schreiner, D. Marx, *Prebiotic Peptide Synthesis on Blue Gene Platforms at Iron-Sulfur-World Conditions* , inSiDE, **6**, 30-35 (2008).

83. E. Schreiner, N. N. Nair, R. Pollet, V. Staemmler, D. Marx, *Dynamical magnetostructural properties of Anabaena ferredoxin* , Proc. Nat. Acad. Sci. USA, **104**, 20725-20730 (2007).

84. N. N. Nair, E. Schreiner, D. Marx, *Glycine at the Pyrite-Water Interface: The Role of Surface Defects* , J. Am. Chem. Soc. **128**, 13815 (2006).

85. K. Jug, N. N. Nair, I. P. Gloriozov, *Molecular Dynamics Study of the Thermal Entropy in Mixed Zinc Chalcogenides ,* J. Phys. Chem. B **110**, 4111 (2006).

86. K. Jug, N. N. Nair, T. Bredow, *Reactions of Surface Hydroxyls with Vanadia on Anatase Surfaces ,* Surf. Sci. **596**, 108 (2005).

87. K. Jug, N. N. Nair, T. Bredow, *Molecular Dynamics Investigation of Water Adsorption on Rutile Surfaces ,* Surf. Sci. **590**, 9-20 (2005).

88. K. Jug, N. N. Nair, T. Bredow, *Molecular Dynamics Investigation of Oxygen Vacancy Diffusion in Rutile ,* Phys. Chem. Chem. Phys. **7**, 2616-2621 (2005).

89. N. N. Nair, T. Bredow, K. Jug, *Towards an Understanding of VOx/TiO2 Catalyst Formation ,* J. Phys. Chem. B **109**, 12115-12123 (2005).

90. N. N. Nair, T. Bredow, K. Jug, *Molecular Dynamics Implementation in MSINDO: Study of Silicon Clusters ,* J. Comput. Chem. **25**, 1255-1263 (2004).

Conference Papers:

1. S. Venkatesan, Sooraj K., Nisanth N. Nair, Sumit Basu *Coarse grained molecular dynamics simulations on the uniaxial stress strain response of PMR 15 ,* 2012

SAMPE International Symposium and Exhibition - Emerging Opportunities: Materials and Process Solutions; Baltimore, MD; United States

2. Sooraj K., Nisanth N. Nair *Mechanism of oxidative degradation of PMR-15 ,* 2012 SAMPE International Symposium and Exhibition - Emerging Opportunities: Materials and Process Solutions; Baltimore, MD; United States

3. J. H. Franke, Nisanth N. Nair, L. Chi, H. Fuchs *Constrained density functional theory of molecular dimers ,* High Performance Computing in Science and Engineering 2011 - Transactions of the High Performance Computing Center, Stuttgart, HLRS 2011, Pages 169-183