Santo Kolattukudy Poulose (Kolattukudy P. Santo)

133 Barnt Ave, Trenton, NJ, USA, 08611 +17325436508 DOB: 18th October 1977 <u>santotheophys@gmail.com,</u> <u>santo.kolattukudy@rutgers.edu</u> https://sites.google.com/site/kpsantobiophys/ Google scholar citations: 490+

PROFESSIONAL SUMMARY

I am an expert in theoretical and computational research of soft materials. Soft materials are classified as materials that easily deform when a force is applied. Examples include biomatter, polymers, colloids, liquids, and nanomaterials. My research encompasses a wide range of topics, including biomolecules, proteins, lipid membranes, viruses such as SARS-CoV-2 and bacteriophages, polymers, metal-polymer complexes, polymer brushes, polysaccharides, polyelectrolyte membranes, colloidal systems, surfactants, shock waves, energy adsorption systems, chromatographic separation, and electron beam lithography. I am proficient in several computational scientific software packages, scientific programming, and source code modifications. I have experience teaching physics and computational methods to master's and graduate students. I have collaborated with expert researchers and students from around the globe, including India, Canada, the USA, Africa, Russia, and China. I have successfully secured research grants from funding agencies such as the National Science Foundation, the New Jersey Alliance of Clinical and Translational Medicine (NJACTS), and have worked on projects with industry partners such as DuPont and Colgate-Palmolive

EDUCATION

PH.D. Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India. 2007

Thesis title: *Theoretical Investigations on a few Biomolecular Rate processes*Adviser: Dr. Kizhakeyil Lukose Sebastian
MSC. PHYSICS. Cochin University of Science and Technology, Kochi, Kerala, India.
2000
First class with distinction and second rank
Thesis title: *Quantum Indistinguishability and a Two-level Bose system*Adviser: Dr. Ramesh Babu T
BSC. PHYSICS. Mahatma Gandhi University, Kottayam, India
1997

First class with distinction (Marks: 88.5%)

EXPERIENCE

RESEARCH ASSISTANT PROFESSOR. Department of Chemical and Biochemical Engineering, Rutgers University, New Brunswick, NJ. USA. September 2022- Present

POSTDOCTORAL ASSOCIATE, Department of Chemical and Biochemical Engineering, Rutgers University, New Brunswick, NJ. USA. 2015-2022

Supervisor: Alexander Neimark

POST DOCTORAL RESEARCH ASSOCIATE, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, USA. 2011-2014

• Supervisor: Max Berkowitz

POST-DOCTORAL FELLOW AND VISITING SCIENTIST, University of Alberta, Edmonton, Canada & National Institute of Nanotechnology, NRC, Canada. 2007-2010.

• Supervisors: Maria Stepanova, Andry Kovalenko.

PROJECTS

A. Ongoing projects: Role – Senior Personnel, Rutgers University, New Brunswick

1. Coarse-grained modeling of surfactant and amino acid adsorption of dental biofilms -Colgate Palmolive; PI Alexander Neimark

• Development computational models of dental biofilms and the adsorption of surfactants and amino acids that are constituents of oral care products.

2. Multiscale Modeling of Coronavirus Virions in the Respiratory System, NSF DMR – 2138052 (2022-); PI. Alexander Neimark

• Development of models of interactions of Coronaviruses with lung surfactants.

3. Development of Computational Models to Explore Interactions of Coronavirus Virions with Lung Surfactant Films, NJ ACTS Pilot Project Grant Program (2021-2022); PI. Alexander Neimark

• Development of models of interactions of Coronaviruses with lung surfactants.

4. Collaborative Research: Interactions of Airborne Engineered Nanoparticles with Lung Surfactant Films, NSF-CBET 2040302 (2020-2023); PI. Alexander Neimark

• Development of coarse-grained computational models of interactions of lung surfactant and engineered nanoparticles.

B. Completed projects. Role- Senior Personnel, Rutgers University, New Brunswick

5. Colgate Palmolive project: Computational Modeling of Xanthan Gum Solutions; PI. Alexander Neimark

 Developed all-atom and dissipative particle dynamics (DPD) models of Xanthan gum (XG), and analyzed conformational and rheological behavior of Zinc-Xanthan systems, phosphoric acid-Zinc-Xanthan gum systems and pH effects on XG conformations.

6. Molecular Design of Biomimetic Lipid Membranes and Liposomes, Rutgers Bush Biomedical Award; PI. Alexander Neimark

• Developed models of interactions between lipid membranes with surfaces and nanoparticles.

C. Completed projects. Role-Post doctoral associate, Rutgers University, New Brunswick

7. GOALI: Theoretical Foundations of Interaction Nanoparticle Chromatography NSF - CBET(510993); PI. Alexander Neimark

• Developed theoretical foundations of interaction nanoparticle chromatography (INPC) by performing DPD simulations and theoretical analysis.

8. Adhesion and Translocation of Nanoparticles through Lipid Membranes NSF – CBET (1264702); PI. Alexander Neimark

Development of models of interactions between lipid membranes with surfaces and nanoparticles.

9. Mass Transport, Kinetics, and Catalytic Activities of Multicatalyst Polyelectrolyte Membranes DTRA (HDTRA1-14-1-0015); PI. Alexander Neimark

- Develop DPD models of metal-complexation on structural, transport and rheological behavior in polyelectrolyte solutions and membranes, mentor graduate students, prepare manuscripts for publications and present results in conferences.
- 10. American Chemical Society Petroleum Research Fund (ACS-PRF), grant No. 54610-ND6; PI. Aleksey Vishnyakov
 - Develop models of asphaltene aggregations in crude oil, mentor undergrad students, prepare manuscripts for publications and present results in conferences.

D. Completed projects. Role-Post doc, University of North Carolina at Chapel Hill.

- 11. Grant No. N00014-14-1-0241 -Office of Naval Research. PI. Max Berkowitz
 - Coarse-grained molecular dynamics simulations of shock wave -cell membrane interactions; wave propagation, collapse of nanobubbles near a lipid membrane, and membrane damage.
- 12. NSF grant No. MCB-0950280 PI. Max Berkowitz

• Perform coarse-grained simulations of action of antimicrobial peptides with model cell membranes, mentor graduate students, prepare manuscripts for publications and present results in conferences.

D. Completed projects. Role-Post doc, University of Alberta, Edmonton, AB, Canada

13. Grant: National Research Council (NRC), Canada PIs. Maria Stepanova, Andriy Kovalenko

- Development of self-consistent field theory (SCFT) of morphological behavior of surfactant assembly at air-water interfaces *Developed:* Code (c++) for running 3D SCFT simulations.
- 14. Grant: NINT-NRC and Alberta Prion research Institute PIs. Maria Stepanova, David Wishart

• Perform simulations of essential collective dynamics of prion protein conformations and compare with NMR data.

15. Grant: NRC-NINT, NSERC, Alberta Innovates, Alberta Advanced Education and Technology (AAE&T), and iCORE PIs. Maria Stepanova, Steven Dew

• Development of atomistic simulation models of interactions of polymer fragments with developer solutions in electron beam lithography and compare with experimental data.

E. Works as graduate student at Indian Institute of Science, Bengaluru, India

1. Rate process involving polymer chains. PI. K. L. Sebastian

• Study rate processes involving single linear polymer chains using theoretical statistical mechanical methods and theories of rate processes. *Developed*. An original theoretical formalism for describing, semiflexible polymers and their loop formation and opening dynamics, a model for kinetics of packaging of DNA in viral capsids, a model for adsorption assisted translocation of proteins across different organelles in the cell.

F. Projects for computer resources-Rutgers university.

<u>XSEDE</u>

1. Building theoretical foundations of nanoparticle chromatography with mesoscale simulations (2017). Role: PI

2. Building theoretical foundations of nanoparticle chromatography with mesoscale simulations-supliment request (2018). Role: Co-PI

3. Deformation of Poroelastic Nanoporous Materials of Hierarchical Structure upon Adsorption of Gas Mixtures (2020). Role. PI

4. Interactions of Airborne Engineered Nanoparticles with Lung Surfactant Films (2022). Role: PI

Anton-2

5. A computer time of 230000 MD units was awarded for studying coronavirus interactions in the respiratory system using microsecond long molecular dynamics simulations. (2022-2023). Role Co-PI.

TEACHING AND MENTORING EXPERIENCE

GUEST FACULTY OF THEORETICAL PHYSICS, Department of Physics, Central University of Kerala, Nileshwar, Kerala, India. 2014-2015

 Courses Taught: PHY 513-Classical electrodynamics, PHY524-Computational physics, PHY5025 -Soft matter Physics.

TEACHING ASSISTANT: Rutgers University. 16:155:513 Fundamentals of Nanoscale Thermodynamics and Transport (by Alexander Neimark) 2019

• Role: Developed computational modules for the graduate course "Nanoscale Thermodynamics and Transport", guided students, presented practice sessions.

Mentored Students: Total 13. Undergraduates-4, Master Students-3, Graduate students-5, Postdocs -1

PEER-REVIEWING EXPERIENCE

Total Reviews: 33

Journal of Molecular Liquids -1, Soft Matter -4, Macromolecular Theory and Simulations -1, Current Opinion in Colloid and Interface Science -1, RSC Advances -3, Applied Surface Science -2, The Journal of Physical Chemistry -7, Langmuir-1, Chemical Reviews -2. Molecular System Design & Engineering -2, Journal of Colloid and Interface Science -2, Physical Chemistry Chemical Physics -1, Minerals -1, Journal of chemical physics-5.

SKILLS

- Linux
- Windows
- C++
- Fortran
- Bash
- Python

Theory of

polymers

- Molecular Dynamics simulations (MD)
- Coarse-grained simulations (CGMD)
- Dissipative particle Dynamics (DPD)
- Brownian/Langevin Dynamics
- High performance computing (LLNL, Anton2, XSEDE)
- Statistical Mechanics

- AMBERGROMACS
- LAMMPS
- DL_MESO
- NAMD
- Materials
 - Studio
- MATLAB
- MATHEMATICA
- Chemsketch
- PoreBlazer
- VMD
- Blender
- LaTex
- Chemsketch
- Chimera
- GnuPlot
- Path Integrals
- Chemical Dynamics theory

PUBLICATIONS

A. JOURNAL ARTICLES (Cover pages 4).

1. Adsorption of Pulmonary and Exogeneous Surfactants on SARS-CoV-2 Spike Protein. **K. P Santo** and A. V, Neimark. *J. Colloid Interface Sci.* (2023) (preprint bioRxiv 2022: <u>https://doi.org/10.1101/2022.05.04.490631</u>)

2. The effects of multiparticle interactions on the aggregation of asphaltenes. I. Kopanichuk, **K.P Santo** and A. Vishnyakov. (*Colloids and Surfaces* A, **636**, 128026, 2022)

3. Dissipative Particle Dynamics in Colloid and Interface Science: A Review. **K. P. Santo** and A. V. Neimark. *Advances in Colloid and Interface Science*, **298**,102545 (2021).

4. Modeling of the effects of metal-complexation on morphology and rheology of Xanthan Gum polysaccharide solutions. **K. P. Santo**, K. Fabijanic, C-Y. Chung, A. Potanin and A. V. Neimark. *Macromolecules*, **54**, 8675-8692, (2021)

5. Effects of Metal-Polymer Complexation on Structure and Transport Properties of Metal-Substituted Polyelectrolyte Membranes. **K. P. Santo**, and A.V. Neimark. *Journal of Colloid and Interface Science*, **602**, 654-668 (2021)

6. Stability of Lipid Coatings of Nanoparticle Coated Surfaces. Parva Patel. **K. P Santo,** S. Burgess, A.Vishnyakov and A. V. Neimark. *ACS nano*, **14**, 17273-17284 (2020)

7. Modeling Gas-Liquid Interfaces by Dissipative Particle Dynamics: Adsorption and Surface Tension of Cetyl Trimethyl Ammonium Bromide at Air-Water Interface. X. Wang, **K** .**P. Santo**, and A. V. Neimark. *Langmuir*, **36**, 14686-14698, (2020)

8. Nanoparticles Flow in Polymer -grafted channel. S. Burgess, **K. P. Santo**, Y. Brun and A.V. Neimark. *Journal of Physical Chemistry C*, **124**, 1478-1483 (2020)

9. Reversible aggregation of particles with short oligomeric sidechains at the surface studied with Langevin dynamics. **K. P. Santo** and A. Vishnyakov, *Colloids and Surfaces A*, **586**, 124143 (2020)

10. Critical Conditions of Adhesion and Separation of Functionalized Nanoparticles on Polymer Grafted Substrates. **K. P.** Santo, A, Vishnyakov, Y. Brun and A.V. Neimark. *Journal of Physical Chemistry C*, **123**, 26, 16091-16106 (2019)(Featured on Cover)

11. Elucidating the effects of metal-complexation on morphological and rheological properties of polymer solutions by a dissipative particle dynamics model. **K. P Santo**, A. Vishnyakov, R. Kumar and A.V. Neimark. *Macromolecules* **51**, 4987-5000 (2018). (*Featured on cover*)

12. Adhesion and Separation of Nanoparticles in polymer –grafted porous substrates. **K. P. Santo**, A, Vishnyakov, Y. Brun and A.V. Neimark. *Langmuir*, **34**,1481–1496 (2018). (*Featured on cover*)

13. Local pressure changes in lipid bilayers due to adsorption of melittin and magainin-h2 antimicrobial peptides: Results from computer simulations. A. Goliaei, **K. P. Santo** and M. L. Berkowitz. *J. Phys. Chem. B*, **118**, 12673-12679 (2014).

14. Shock wave- induced collapse of arrays of nanobubbles located next to lipid membrane: Coarse-grained computer simulations. **K. P. Santo** and M. L. Berkowitz. *J. Phys. Chem. B*, **119**, 8879–8889 (2015).

15. Shock wave interaction with a phospholipid membrane: Coarse-grained computer simulations. **K. P. Santo** and M. L. Berkowitz, J. Chem. Phys. **140**, 054906, (2014)

16. Melittin creates transient pores in a lipid bilayer: Results from computer simulations. **K. P. Santo**, S. J. Irudayam and M. L. Berkowitz, *J. Phys. Chem. B*, **117**,5031-5042(2013).

17. Difference between Magainin-2 and Melittin Assemblies in Phosphatidylcholine Bilayers: Results from Coarse-Grained Simulations. **K. P. Santo** and M. L. Berkowitz, *J. Phys. Chem. B*, **116**, 3021–3030 (2012).

18. Study of the interaction of polymethylmethacrylate fragments with methyl isobutyl ketone and isopropyl alcohol. M. A. Mohammad, **K. P. Santo**, S. K. Dew and M. Stepanova, *J. Vac. Sci. Technol. B*, **30**, 06FF11 (2012).

19. Comparative analysis of essential collective dynamics and NMR-derived flexibility profiles in evolutionarily diverse prion proteins. **K. P. Santo**, M. Berjanskii, D. S. Wishart and M. Stepanova, *Prion*, **5**, 188 - 200 (2011)

20. Self-consistent field modeling of the three dimensional morphologies of branched lipid surfactant at air-water interface. **K. P. Santo**, A. Kovalenko and M. Stepanova, *Macromol. Theor. Simul.* **19**, 228, (2010) (*featured on cover*)

21. Dynamics of loop formation in a semiflexible polymer. K. P. Santo and K. L. Sebastian, Phys. Rev. E, 80, 061801 (2009).

22. Opening of a Weak link in a semiflexible Ring polymer. K. P. Santo and K. L. Sebastian, Phys. Rev. E, 73, 031923 (2006).

23. Simple model for kinetics of packaging of DNA into a capsid against an external force. **K. P. Santo** and K. L. Sebastian, *Phys. Rev. E*, **65**, 052902 (2002).

B. CONFERENCE ORAL PRESENTATIONS (Presenter underlined)

13. Selective Adsorption of Surfactants on Coronavirus Virions. <u>A.V. Neimark</u>, K.P. Santo, AIChE annual meeting, Phoenix, AZ, November 13-18, 2022.

12. Exploring surfactant adsorption on SARS-CoV-2 Spike protein by coarse-grained molecular dynamics simulations. K. P Santo and A. V. Neimark. ACS Fall 2022, August 22, Chicago, IL, USA,

11. Modeling of the Effects of Addition of Zinc on Morphology and Rheology of Xanthan Gum Polysaccharide Solutions. <u>K. P Santo</u>, A. Potanin and A. V. Neimark ACS Fall 2021, August 23 2021, Atlanta GA, USA.

10. Morphological and Transport Properties of Metal-complexed Polyelectrolyte Membranes. <u>K. P Santo</u> and A.V Neimark, ACS Fall 2021, August 24 2021, Atlanta GA, USA.

9. Interaction nanoparticle chromatography on polymer grafted substrates at critical conditions of adsorption<u>. K.P Santo</u>, A. Vishnyakov, Y. Brun and A.V. Neimark. 93rd ACS Colloid & Surface Science Symposium, Georgia Tech, Altanta June 18, 2019

8. Morphological and rheological properties of metal-complexed polymer solutions studied using a dissipative particle dynamics model. <u>K.P. Santo</u>, A. Vishnyakov, R. Kumar and A.V. Neimark 92nd ACS Colloid & Surface Science Symposium, 12th June 2018, Penn Stater Hotel and Conference Center, State College, PA, USA.

7. Separation of functionalized nanoparticles on polymer-grafted porous substrates. <u>K.P. Santo</u>, A. Vishnyakov, Y, Brun and A.V. Neimark. 92nd ACS Colloid & Surface Science Symposium, 12th June 2018, Penn Stater Hotel and Conference Center, State College, PA, USA.

6. Colloidal Aggregation of Asphaltenes Studied through Computer Simulations. <u>K.P. Santo</u> and A. Vishnyakov. 91st ACS Colloid & Surface Science Symposium, 12th July 2017, The City College of New York, New York, USA

5. Adhesion and Separation of Nanoparticles in Polymer-grafted porous substrates. <u>K.P. Santo</u>, A. Vishnyakov, Y, Brun and A.V. Neimark. 91st ACS Colloid & Surface Science Symposium, 10th July 2017, The City College of New York, New York, USA.

4. Structural and thermodynamic characteristics of melittin-phospholipid bilayer interaction: Results from computer simulations. <u>M. Berkowitz</u>, S. Irudayam, K. Santo and R. Vacha. 245th ACS National meeting (2013), New Orleans, LA, USA.

3. Comparative analysis of prion proteins for evolutionarily diverse vertebrate species, polymorphic variants and mutants-Structure and essential dynamics. <u>M. Stepanova</u>, B. Issack, K. Santo, T. Fito, M. Berjanskii, D. Wishart. Prion meeting 2012

2. Exploring the Conformational Dynamics of Prion Proteins to Understand the Mechanism of Susceptibility/Resistance to Pathological Conversion. <u>Bilkiss B. Issack</u>, K. P. Santo, Taras Fito, Mark Berjanskii, David S. Wishart, and Maria Stepanova. PRION meeting (2011)

1. Surfactant self-assembly in Three-dimensions. K. P. Santo, A. Kovalenko and <u>M. Stepanova</u>, Proceedings of the 8thWorld Congress on Chemical Engineering (WCCE8), August 23-27, Montreal, Canada, 2009

C. CONFERENCE POSTER PRESENTATIONS (Presenter underlined)

26. Acoustic force spectroscopy reveals subtle differences in interfacial protein-polysaccharide binding interactions. <u>Shishir</u> <u>P. S. Chundawat</u>, Markus Hackl, Cesar Lopez, Kolattukudy P. Santo, Sandrasegaram Gnanakaran, Alexander Neimark, , Biophysical Society Meeting, Philadelphia, PA, February 10-14 2024.

25. Dissipative Particle Dynamics Modeling of Phospholipid Monolayers at Air-Water Interfaces: Temperature-Dependent Two-Dimensional Phase Behavior and Elastic Properties. <u>Kolattukudy P. Santo</u>, Monica Iepure, Yuanzhong Zhang, Younjin Min, and Alexander V. Neimark, Biophysical Society Meeting, Philadelphia, PA, February 10-14 2024.

24. Adsorption of pulmonary surfactants on the spike proteins of SARS-CoV-2 and its variants. <u>Kolattukudy P. Santo</u>, Ryan Jaworski and Alexander V. Neimark, Biophysical Society Meeting, Philadelphia, PA, February 10-14 2024.

23. Adsorption of Pulmonary Surfactants on SARS-CoV-2 Spike Protein. <u>Ryan Jaworski</u>, Kolattukudy Santo, Alexander Neimark. RISE research symposium, 2023, Rutgers University, Piscataway, NJ, USA, August 2, 2023

22. Nanoscale energy adsorption systems: pressure-driven intrusion and extrusion of water in hydrophobic nanopores. <u>Abdelraheem Abdallah</u>, Kolattukudy P. Santo, and Alexander V. Neimark. 4th Molecular Simulations Workshop, New Jersey Institute of Technology, Newark, NJ, USA, May 30 2023.

21. Colloidal Aggregation of Asphaltenes Studied with Brownian Dynamics and Monte Carlo Simulations. <u>F. Taherkhani</u>, A Vishnykov, Kolattukudy P. Santo. XXII International Conference on Chemical Thermodynamics in Russia (2019)

20. Modeling of the Effects of Addition of Zinc on Morphology and Rheology of Xanthan Gum Polysaccharide Solutions. <u>K.</u> <u>P Santo</u>, A, Potanin and A.V. Neimark. Sci-Mix Poster, ACS Fall 2021, August 23 2021, Atlanta GA, USA.

19. Nanoparticle separation in polymer-grafted porous substrates. <u>K. P. Santo</u>, A.Vishnyakov, Y. Brun and A.V. Neimark. 8th Characterization of Porous Materials (CPM8) Conference, Delray Beach Marriot, Delray Beach, Florida, USA, May 6-9, 2018.

18. Effects of shock wave-induced collapse of nanobubbles near lipid membranes. <u>K. P. Santo</u> and M.L. Berkowitz. First Annual Research Computing Symposium, University of North Carolina Chapel Hill, Alumni Hall III, Carolina Club, May 20, 2014.

17. Shock wave-induced damage of lipid membranes in the proximity of single or multiple nanobubbles. <u>K. P. Santo</u> and M.L. Berkowitz. Triangle soft matter workshop, May 8 2014, Murray Hall, University of North Carolina and Chapel Hill, Chapel Hill, NC. USA.

16. Coarse-grained simulations of antimicrobial action of Melittin and Magainin-2 on phospholipid bilayers. <u>K. P. Santo</u> and M. L. Berkowitz, Biophysical Society 57th Annual Meeting, February 2-6, (2013), Philadelphia, Pensilvania, USA.

15. Study of of the Interaction of Polymethylmethacrylate Fragments with Methyl Isobutyl Ketone. M. A. Mohammad, <u>K. P. Santo</u>, S. K. Dew, M. Stepanova, The 56th International Conference on Electron, Ion and Photon Beam Technology and Nanofabrication (EIPBN) 2012. Waikoloa, Hawai, USA..

14. Collective dynamics in prion proteins: a comparative analysis of disease-prone and disease-resistant species. <u>K. P.</u> <u>Santo</u>, M. Berjanskii, D. S. Wishart, and M. Stepanova, The 17th Canadian Symposium on Theoretical Chemistry (CSTC 2010), July 25-30, Lister Center, University of Alberta, Edmonton, Canada.

13. Three-dimensional morphologies of lipid surfactant studied by self-consistent field modeling. <u>K. P. Santo</u>, A. Kovalenko and M. Stepanova. NanoForum Canada 2008, May 28-29, 2008, Telus Center, University of Alberta, Edmonton, Canada

12. Dynamics of loop formation in Semiflexible polymers. <u>K. P. Santo</u> and K. L. Sebastian, The First Asian spectroscopy conference, 29 th January to 2nd February (2007), Indian Institute of Science, Bangalore, India.

11. Theory of loop formation in semiflexible polymers. <u>K. P. Santo</u> and K. L. Sebastian. Chemical division day, 21st January (2007) Indian Institute of Science, Bangalore, India.

10. Opening dynamics of a Semiflexible Polymer Ring. <u>K. P. Santo</u> and K. L. Sebastian, Workshop on biopolymers: Thermodynamics, Kinetics and Mechanics of DNA, RNA and Proteins, May 30th to June 3rd (2005), The Abdus Salam International Center for theoretical Physics, Trieste, Italy.

9&8. (a) A Simple Model for Kinetics of Packaging of DNA into a Viral Capsid against an External Force. (b) Opening of a Semiflexible Polymer Ring . <u>K. P. Santo</u> and K. L. Sebastian. STATPHYS -22, The 22nd International Conference on Statistical Physics, July 4-9, (2004), Indian Institute of Science, Bangalore, India.

7&6. (a) Kinetics of DNA Packaging into a Viral Capsid against an External Force. (b) Dynamics of Semiflexible Polymer loops: Rate of Opening. <u>K. P. Santo</u> and K. L. Sebastian. The DAE-BRNS Symposium on Theoretical Chemistry, December 9-12,(2004), Bhabha Atomic Research Center, Mumbai, India.

5&4. (a) A Simple Model for Kinetics of Packaging of DNA into a Viral Capsid against an External Force. (b) Opening of a Semiflexible Polymer Ring. <u>K. P. Santo</u> and K. L. Sebastian, International symposium on molecules, machines and networks, January 6-9, (2004), National Centre for Biological Sciences (NCBS), Bangalore, India.

3. Opening of a Semiflexible Polymer Ring. <u>K. P. Santo</u> and K. L. Sebastian. In-house Symposium,(2003), Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India.

2. A Simple Model for Kinetics of Packaging of DNA into a Viral Capsid against an External force. <u>K. P. Santo</u> and K. L. Sebastian. In-house Symposium, (2002), Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India (second best poster award).

1. A Simple Model for Kinetics of Packaging of DNA into a Viral Capsid against an External force. <u>K. P. Santo</u> and K. L. Sebastian. India and Abroad: Conference on condensed matter Physics, January 2-4, (2002), Jawaharlal Nehru Centre for Advanced Scientific Research and Indian Institute of Science, Bangalore, India

OTHER TALKS

15. *Computer Simulations of some Nanoparticle systems.* Prof. Priya Vashishta's Group, University of Southern California, Los Angeles. February 14, 2017.

14. *Collapse of Nanobubbles by a Shock wave near Lipid membranes: Coarse-grained simulations.* Department of Physics, Indian Institute of Science Education and Research (IISER), Bhopal, Indian, 16th September 2014.

13. *Effects of shock wave -induced collapse of a nanobubble and nanobubble arrays near lipid membranes.* Department of Physics, Cochin University of Science and Technology, Kochi, Kerala, India, 17th July 2014.

12. *Shock wave-induced collapse of nanobubbles near lipid membranes: Coarse-grained molecular dynamics simulations.* Department of Inorganic and physical chemistry, Indian Institute of Science, Bangalore, India, 10th July 2014.

11. *Analysis of structural stability and back-bone flexibility in disease-prone and disease resistant prion proteins*. The Prion Group, University of Alberta, Canada, May 7th 2010.

10. *Self Assembly of Amphiphilic Lipids at Air-Water Interface: A Three-Dimensional Self-Consistent field modeling.* Biophysics Journal Club, Department of Physics, University of Alberta, Edmonton, Canada, December 1, 2009.

9. Surfactant Self-Assembly in three-dimensions: A Self-Consistent field modeling. Special lecture, organized by Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India and Royal Society of Chemistry (Decan section, India), 15th July, 2009.

8. Exploring Nano Science. Sacred Heart College, Chalakudy, Kerala, India, August 18, (2009).

7. *An SCFT Study on Surfactant Self-assembly in Three-dimensions.* Theory and modeling group, National Institute of Nanotechnology, University of Alberta, Edmonton Canada, 8th April 2009.

6. *Modeling of PMMA resist-developer interaction in electron beam lithography: Studies by RISM and molecular dynamics.* Theory and modeling group, National Institute of Nanotechnology, University of Alberta, Edmonton Canada, 26th November 2008.

5. *Statistical mechanical studies of a few single chain processes and 3D simulation of the phase behavior of DPPC at airwater interface.* Theory and modeling group, National Institute of Nanotechnology, University of Alberta, Edmonton, Canada, 24th January 2008.

4. *Theoretical Investigations on a few Biomolecular Rate Processes.* Thesis colloquium, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India, 26 th May, 2006.

3. *The Geometrical Approach to protein Folding.* Department of Inorganic and Physical Chemistry, Indian Institute of Science, 2003.

2. *Simple Model for Kinetics of packaging of viral DNA into a Capsid against an external Force.* Department of Inorganic and Physical Chemistry, Indian Institute of Science, 2002.

1. *Theory of Protein Folding: The energy Landscape perspective.* Department of Inorganic and Physical Chemistry, Indian Institute of Science, 2002

PROFESSIONAL MEMBERSHIPS

American Chemical Society (ACS) member Biophysical Society (BPS) annual member

AWARDS

Second rank, MSc. Physics (2000) Cochin University of Science & Technology, Kochi, India Junior Research Fellowship (1999), Council of Industrial and Scientific Research (CSIR) India. Junior Research Fellowship (1999), University Grants Commission (UGC) India. Second Best poster Award (2002), Inhouse Symposium, Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, India.

Senior Research Fellowship (2003), Council of Industrial and Scientific Research (CSIR) India.