RESUME

Department of Physics
Indian Institute of Technology Jodhpur
NH 65, Nagaur Road Karwar, Jodhpur 342037, INDIA
Phone: (0291) 280-1613; eMail: santosh@iitj.ac.in

SANTOSH MOGURAMPELLY
Assistant Professor

MULTISCALE MODELING OF SOFT MATTER PHYSICS

Objective: I am a highly motivated researcher having more than 12 years of experience in fundamental and applied scientific research with a strong academic training in physics. I specialize in the development and application of **multiscale modeling approaches** including the first principle Density Functional Theory (DFT) calculations, ab-initio to classical level MD simulations and coarse-grained methods. I used DFT methods to calculate electrostatic charges, binding energies, vibrational spectra, potential energy scans and develop classical level force field parameters. I also develop and use multiscale MD simulations (ab-initio, atomistic and coarse-grained) to investigate a broad range of problems in **polymer physics, materials science and engineering**. In the past, I have contributed significantly to the advancement of Li-ion polymer batteries, 2D materials and body-armor applications and consistently published research outcomes in top-tier journals like JACS, JPC Letters, ACS Macro Letters, Nanoscale, Physical Review Materials and Macromolecules. At the IIT Jodhpur, I aim to promote a competitive environment as a computational researcher and determined to focus on high quality teaching as well as cutting-edge research towards realizing technological applications.

EDUCATION, TRAINING AND EXPERIENCE

TEMPLE UNIVERSITY — **PHILADELPHIA, PA, USA**
POSTDOCTORAL RESEARCH FELLOW — **2016-2019**
Research Theme: *Advanced Materials Modeling for Body-armor Applications*; Advisor: Prof. Michael L Klein

- Projects: Force field development, fiber formation of Kevlar®/UHMWPE complexes and nanocomposites.
- Coarse-grained potential model development and large-scale MD simulations of Kevlar® fiber formation.
- Density Functional Theory (DFT) & first principle MD simulations for organic molecules and liquids.
- Extensive collaboration with experimental groups for composites, organic molecules, batteries and NMR.
- Presented research results in national and international conferences.

THE UNIVERSITY OF TEXAS AT AUSTIN — **AUSTIN, TX, USA**
POSTDOCTORAL RESEARCH FELLOW — **2014-2016**
Research Theme: *Ion Transport Studies in Polymer Electrolytes for Batteries*; Advisor: Prof: Venkat Ganesan

- Projects: Polymer nanocomposites, ternary electrolytes, ionic liquids and polymerized ionic liquids
- Developed force fields using DFT and conducted atomistic MD simulations. Developed kMC tool.
- Designed and mentored multiple undergraduate and graduate research projects for Li-ion batteries.
- Presented research results in national and international conferences.

THE UNIVERSITY OF ROME "LA SAPIENZA" — **ROME, ITALY**
POSTDOCTORAL RESEARCH FELLOW — **2012-2013**
Research Theme: *Developing Computational Model for a Bundle of Filaments*; advisor: Prof: Giovanni Ciccotti

- Developed a hybrid simulation model consisting GCMC, reaction MC and Brownian Dynamics
- Designed and mentored an undergraduate research project.

TECHNICAL UNIVERSITY MUNICH — **MUNICH, GERMANY; AUG-DEC 2010**
Internship Project: *Elasticity of DNA and the effect of dendrimer binding*; Advisor: Prof. Roland R. Netz

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INDIAN INSTITUTE OF SCIENCE (IISC) — **BANGALORE, KARNATAKA, INDIA**
PHD, COMPUTATIONAL PHYSICS — **2007-2012**
Thesis: *Elasticity and Structural Phase Transitions of Nanoscale Objects*; Advisor: Prof. Prabal K Maiti

- Projects: Elasticity of boron nitride nanotubes, carbon nanotubes, DNA, RNA and Dendrimers; Interaction of nanomaterials with soft matter systems.
- DFT calculations for electrostatic charge assignment and binding energies.
- Atomistic MD simulations of nanomaterials and bio-polymers.
- Teaching assistant for Molecular Simulations course for two semesters
- Delivered (oral and poster format) numerous presentations within India and abroad.

UNIVERSITY OF HYDERABAD — **HYDERABAD, TELANGANA, INDIA**
MSC, PHYSICS — **2004-2006**

KAKATIYA UNIVERSITY — **HANMAKONDA, TELANGANA, INDIA**
BSC (MATHEMATICS, PHYSICS AND COMPUTER SCIENCE) — **2001-2004**

AWARDS AND FELLOWSHIPS

- ERASMUS MUNDAS fellowship in 2010 for internship at Technical University Munich, Germany.
- Best poster award in 2009 at the in-house symposium of Department of Physics, IISc, Bangalore.
- Senior Research Fellowship in 2009 & Junior Research Fellowship in 2006 awarded by CSIR.
- Qualified GATE and JEST in 2006.

TECHNICAL SKILLS

- Expertise with Gaussian, Quantum Espresso, Schrodinger, Materials Studio, MATLAB, Mathematica, LAMMPS, AMBER, NAMD, Jaguar, VMD etc.
- Experience in FORTRAN, C, C++, Shell scripting, LINUX and Windows.
- Wrote MD codes in various ensembles, *viz.*, NVT, NPT, μVT. Developed a tool to implement kinetic Monte Carlo method. Experience with GPU and optimization of codes with OpenMP & MPI.
- HPC system administration of 10 TFLOP and 4 TFLOP computing clusters at IISc, Bangalore.

MENTORSHIP AND TEACHING EXPERIENCE

- Electromagnetism and Optics (PH111 Summer 2019 along with Prof. Prabhat K Jaiswal): For BTech first year students.
- Computational Materials Science (PHL7310 July-Dec 2019): For Masters and PhD Students.
- General Physics Laboratory (PHP1010 July-Dec 2019): For BTech first year students.
- Social Connect & Responsibilities (OSN1010 July-Dec 2019): For BTech first year students.
- Mentoring three Master students and two PhD students at IIT Jodhpur
- Mentored multiple PhD theses at The University of Texas at Austin, Austin, United States. I played a key role in designing the projects, analyzing the results and writing papers. The research outcomes are published in 5 high quality journals.
- Co-mentoring a PhD thesis at IIT Madras. One paper published and few papers in preparation.
- Designed & mentored two undergraduate projects during my postdoctoral stay at Rome and Austin.
- Served as a tutor at a week-long computational workshop at the JNCASR.
- Teaching assistance for PhD students at the IISc for two semesters in 2009 and 2010.

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SELECTED RECENT PUBLICATIONS

(Full publication list is available at my Google Scholar page: Click Here**)**
IN A NUTSHELL: Total Published Papers: **30**, Book Chapters: **01**, Papers in Review: **03**, Papers in Preparation: **7**
Total citations: **521** (Source-Google Scholar), H-index: **15**, i-10 index: **18**

1. **SANTOSH MOGURAMPELLY**, Jordan R. Keith and Venkat Ganesan, "Mechanisms Underlying Ion Transport in Polymerized Ionic Liquids", *J. Am. Chem. Soc.,* **139**(28), (2017) 9511-9514. (Times cited: 18) IF: 14.357 PDF
2. Zhuolei Zhang, **SANTOSH MOGURAMPELLY (Shared first author)**, Simona Percec, Giacomo Fiorin, Shenqiang Ren and Michael L. Klein, "Mechanically Strong Polymer Sheets From Aligned Ultra-High Molecular Weight Polyethylene Nanocomposites" *J. Phys. Chem. Lett.,* **9**, (2018) 2652-2658. (Times cited: 1) IF: 8.709 PDF
3. **SANTOSH MOGURAMPELLY**, Christopher M. MacDermaid, Simona Percec, Giacomo Fiorin and Michael L. Klein, "Aggregation of Poly(p-phenylene terephthalamide) Chains: Emergence of Fiber Defects" *Phys. Rev. Mater.,* (**Editor's Suggestion**) **3**(1) 015602, (2019). (Times cited: 0) IF: 2.926 PDF
4. **SANTOSH MOGURAMPELLY** and Venkat Ganesan, "Ion Transport in Polymerized Ionic Liquid - Ionic Liquid Blends", *Macromolecules,* **51**(23), (2018) 9471-9483. (Times cited: 0) IF: 5.914 PDF
5. **SANTOSH MOGURAMPELLY** and Venkat Ganesan, "Effect of Nanoparticles on Ion transport in Polymer Electrolytes" *Macromolecules*, **48**(8), (2015) 2773-2786. (Times cited: 29) IF: 5.914 PDF

SELECTED SEMINAR AND POSTER PRESENTATIONS

- Seminar talks in several IITs, CSIR labs, JNCASR, TIFRH and IISc within India.
- 15+ research talks in international conferences & universities in India, USA, Italy and Germany.
- More than 20 poster presentations in India, Italy and USA.

REFERENCES

- **Prof. Michael L. Klein**, Dean of the College of Science and Technology, Temple University, Philadelphia, PA 19122, Email: mlklein@temple.edu
- **Prof. Venkat Ganesan**, Department of Chemical Engineering, The University of Texas at Austin, Email: venkat@che.utexas.edu
- **Prof. Prabal K. Maiti**, Department of Physics, Indian Institute of Science (IISc), India, E-mail: maiti@iisc.ac.in
- **Prof. Dr. Roland R. Netz**, Department of Physics, Freie Universität Berlin, Germany, Email: rnetz@physik.fu-berlin.de