

SANDIPAN CHATTARAJ

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RESEARCH EXPERIENCE

1) IESL-FORTH, Crete, Greece

Postdoctoral Fellowship, November 2025 to present

Topic: Dissipative particle dynamics (DPD) simulations of bio-sourced sustainable colloidal systems

Advisor: Prof. George Petekidis

2) University of Pavia, Italy

Postdoctoral Fellowship, January, 2021 to December, 2024

Topic: Modeling bioengineered tissues with coarse-grained particle dynamics simulations

Advisor: Prof. Francesco Pasqualini

3) IIT Kanpur

Postdoctoral Fellowship, February 2018 to December 2020

Topic: All-atom and coarse-grained molecular dynamics simulations of the polymers, PEEK and PEKK

Advisor: Prof. Sumit Basu

EDUCATION & PROFESSIONAL EXPERIENCE

IIT Bombay, Mumbai, India

PhD, Polymer Science, Nanoscience & Technology, January 2011 to January 2018

Dissertation: Deformation Analyses of Glassy Polymers at Various Length Scales

Advisors: Profs. Hemant Nanavati, Prita Pant, Dnyanesh N. Pawaskar

Tata Consultancy Services, Kolkata, India

Professional Experience, Assistant Systems Engineer, July 2008 - December 2010

Role: Software maintenance for American insurance companies - AIG and 21st Century

Operated on document management system, Documentum (Java)

NIT Durgapur, Durgapur, India

M.Tech., Materials Science, July 2006 to June 2008

Thesis: Electrical Transport Properties of Cu⁺² doped Polyaniline and Polyvinylalcohol

Advisor: Prof. A. K. Meikap

UIT, Burdwan University, Burdwan, India

B.E., Electronics & Communication, July 2002 to June 2006

RELEVANT SKILLS

- Molecular dynamics simulations: LAMMPS, Materials Studio
- Programming in Python, C++, MATLAB, Java
- Optimization, Uncertainty Quantification
- Preparation of crosslinked polymer films and micropillars via photolithography
- Characterization of polymers via optical and electron microscopy, Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC)
- Nanoindentation: thorough knowledge of experimental techniques and data analyses

PUBLICATIONS

1. Saranya Vasudevan, Sandipan Chattaraj, Alessandro Enrico, Francesco Pasqualini, “*Molecular Dynamics Simulation of Structural Assembly and Hydration of Hyaluronic Acid in Salt Aqueous Buffer*”, **Langmuir**, **41** (6) (2025) 3852-3864
2. Sandipan Chattaraj, Michelle Torre, Constanze Kalcher, Alexander Stukowski, Simone Morganti, Alessandro Reali, Francesco Pasqualini, “*SEM²: Introducing mechanics in cell and tissue models using coarse-grained homogeneous particle dynamics*”, **APL Bioengineering**, **7**, 046118 (2023) 1-14
3. Sandipan Chattaraj, Sumit Basu, “*Coarse graining strategies for predicting properties of closely related polymer architectures: a case study of PEEK and PEKK*” **Journal of Materials Research**, **37** (2022) 1-12
4. Sandipan Chattaraj, P. Pant and H. Nanavati, “*Inter-relationships between mechanical properties of glassy polymers from nanoindentation and uniaxial compression*” **Polymer**, **144** (2018) 128-141
5. Sandipan Chattaraj, P. Pant, D. Pawaskar and H. Nanavati, “*How many network chains of a densely crosslinked glassy thermoset deform cooperatively at yield?*” **Polymer**, **82** (2016) 305-318

PRESENTATIONS

1. Oral presentation in **ICAM Workshop 2024**, organized by International Center for Advanced Computing in Medicine. “*SEM²: A Multiscale Model for Cell and Tissue Mechanics in Morphogenesis*” Date: 10 May 2024. Venue: Lugano, Switzerland
2. Oral presentation in **E-MRS Fall Meeting 2019**, organized by European Materials Research Society. “*Coarse-grained molecular dynamics of PEEK and PEKK*” Date: 16-19 September 2019. Venue: Warsaw, Poland
3. Oral presentation in **APS March Meeting 2016**, organized by American Physical Society. “*Molecular Description of Yield in Densely Crosslinked Epoxy Thermosets*” Date: 14-18 March 2016. Venue: Baltimore, USA

RESEARCH INTERESTS

Dissipative Particle Dynamics Simulations of Biosourced Colloidal Systems
Mechanobiology: Modeling bioengineered tissues with particle dynamics simulations
Molecular dynamics simulations of biopolymers
Coarse-graining
Nanoindentation and AFM indentation studies of soft materials

TEACHING INTERESTS

Polymer science and engineering
Mechanical behavior of biomaterials
Molecular dynamics simulations of biomacromolecules
Materials science and engineering