

## Dr. Manjesh Kumar Singh

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## RESEARCH INTEREST

- Soft Matter
- Tribology
- Rheology

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## EDUCATION

### Ph.D. (Materials) (2016)

*Swiss Federal Institute of Technology (ETH Zurich), Switzerland*

### Master of Engineering (Materials) (2011)

*Indian Institute of Science (IISc.), Bangalore, India*

**Grades:** 6.6/8 (First Class)

### Bachelor of Engineering (Mechanical) (2009)

*Bengal Engineering and Science University (Now IEST), Shibpur, West Bengal, India*

**Grades:** 82% (First Class Hons.)

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## Postdoctoral Research

**Supervisor:** Prof. Dr. Kurt Kremer

*Polymer Theory, Max Planck Institute for Polymer Research, Mainz.*

**Research Synopsis:** I am using complementary experimental and simulation approach to study rheology of nonequilibrium disentangled melts of longer polymer chains. The idea is that such systems should display a different rheological behavior, glass transition temperature etc. in comparison to their equilibrated counterparts. The experimental part of the work involves fabrication of single-chain nanoparticles using electrospinning technique, characterizing (using SEM, TEM, AFM and NMR) and investigating the rheological properties, relaxation behavior and glass-transition temperature of disentangled polymer melts consisting of these single-chain nanoparticles. The theoretical part of my research involves performing bead-spring (Kremer-Grest) model based molecular dynamics simulations to prepare fully disentangled melt of globules of single independent chains. Thereafter the disentangled melt is allowed to relax and studied with respect to change in structure of polymer chains (radius of gyration, end-to-end distance and entanglement length), rheological behavior and glass-transition temperature. The development of entanglements during relaxation is studied using primitive path analysis (PPA).

## **PhD Dissertation**

**Supervisor:** Prof. Dr. Nicholas D. Spencer

*Lab for Surface Science and Technology (LSST), Department of Materials, ETH Zurich.*

**Co-supervisor:** Prof. Dr. Martin Kroger

*Polymer Physics Group, Department of Materials, ETH Zurich.*

**Title:** Simulation and Experimental Studies of Polymer Brushes under Shear

**Research Synopsis:** My PhD work involved colloidal probe based AFM experiments and molecular dynamics simulation studies on surface grafted polymer chains (brushes and gels) in a solvent. The main focus of my PhD study was to understand the tribological behaviour of polymer brushes over a range of loads and speeds for different brush architectures and give a design based rule fabrication of polymer brushes with optimal friction and wear properties.

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## **Master Thesis**

**Supervisor:** Prof. Dr. Vikram Jayaram

*Materials Engineering Department, IISc, Bangalore.*

**Co-supervisor:** (Late) Prof. Dr. Sanjay K. Biswas

*Mechanical Engineering Department, IISc, Bangalore.*

**Title:** Simulation and Validation of Roll-Separating Forces and Limiting Reduction in Cold Rolling

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## **WORK**

### **Post PhD Research**

**08/2016 – 09/2019:** Postdoctoral researcher, Polymer Theory, MPIP, Mainz.

**02/2016 – 07/2016:** Postdoctoral researcher, LSST, ETH Zurich.

### **Pre PhD Research**

**09/2011 – 01/2012:** Research Assistant, LSST, ETH Zurich.

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## **SKILLS**

**Programming:** C, Python and Matlab

**Software Packages:** ABAQUS/CAE (FEM), ESPResSo++ and LAMMPS (Molecular Dynamics).

**Instrument Handled:** Atomic Force Microscope, Electrospinning system and Tribometer.

**Languages:** English, Hindi, Bengali and German (A2 level)

**Extra-Curricular:** An enthusiastic runner, participate in different long distance running events, Badminton and Tennis.

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## **TEACHING EXPERIENCE**

- Took practical for undergraduate students on **Atomic Force Microscopy** for 4 semesters.
- Teaching Assistant for the course, **Atomic Force Microscopy in Materials Science**, ETH course number 327-2223-00L held in February 2016

## MEMBERSHIP

- Life member of Tribology Society of India (TSI). Membership number: LM # 5596.
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## CONFERENCES

### Poster Presentation

- Mainz Materials Simulation Days 2017, June 12-14, 2017 at Mainz, Germany. Title: *Relaxation of Disentangled and Collapsed Polymer Chains in a Melt.*
- Soft Smart Responsive Materials: Fundamentals and Applications, May 11-12, 2017 at Mainz, Germany. Title: *Relaxation of Disentangled and Collapsed Polymer Chains in a Melt.*
- Tribology: Interactions Beyond the Surface: A tribute to Prof. Jean-Marie Georges, March 30-31, 2016 at Lyon, France. Title: *Simulation and Experimental Studies of Polymer Brushes under Shear.*
- Gordon Research Conference, July 8-13, 2013 at Waterville, ME, USA. Title: *Modeling studies of interacting Polymer Brushes under Shear.*
- International Nanotribology Forum: The Hoi An Discussions, May 23-27, 2011, Hoi An, Vietnam. Title: *Simulation and Validation of Roll-Separating Forces and Limiting Reduction in Cold Rolling.*
- 7<sup>th</sup> International Conference on Industrial Tribology, Dec. 2-4, 2010 at RDCIS, Ranchi, India.
- 48<sup>th</sup> National Metallurgist Day (NMD), Nov. 14-16, 2010 at Indian Institute of Science, Bangalore, India. Title: *Simulation and Validation of Roll-Separating Forces and Limiting Reduction in Cold Rolling.*

### Contributed Talk

- DPG Spring Meeting 2019, 31 March - 05 April, 2019 at Regensburg, Germany. Title: *Rheology of Nonequilibrium Polymer Melt.*
- DPG Spring Meeting 2018, March 11-16, 2018 at Berlin, Germany. Title: *Relaxation of Disentangled and Collapsed Polymer Chains in a Melt.*
- International Tribology Conference, Sep. 16-20, 2015 at Tokyo, Japan. Title: *Molecular Dynamics Simulation of Crosslinked Polymer Brushes.*
- Swiss-Japanese Tribology Meeting, Sep. 8-10, 2014 at Zurich, Switzerland. Title: *MD Simulation of Polymer Brushes based Tribology.*
- ASIATRIB-2014, Feb. 17-20, 2014 at Agra, India. Title: *Modelling Studies of Interacting Polymer-Brushes under Shear.*
- International Nanotribology Forum: Kerala 2014, Jan. 6-10, 2014 at Kochi, Kerala, India. Title: *Non-equilibrium Molecular Dynamics Simulation of Polymer-Brushes.*
- 5<sup>th</sup> World Tribology Congress, Sep. 8-13, 2013 at Torino, Italy. Title: *Combined Experimental and Simulation studies of Polymer Brushes under Shear.*

## LIST OF PUBLICATIONS

- *Combined Experimental and Simulation Studies of Cross-Linked Polymer Brushes under Shear*; **Manjesh K. Singh**, Chengjun Kang, Patrick Ilg, Rowena Crockett, Martin Kröger and Nicholas D. Spencer; *Macromolecules* **2018**, 51 (24), 10174-10183.
- *Effect of Crosslinking on the Microtribological Behavior of Model Polymer Brushes*; **Manjesh K. Singh**, Patrick Ilg, Rosa M. Espinosa-Marzal, Martin Kröger and Nicholas D. Spencer; *Tribol. Lett.* **2016**, 63, 17.
- *Influence of Chain Stiffness, Grafting Density and Normal Load on the Tribological and Structural Behavior of Polymer Brushes: A Nonequilibrium-Molecular-Dynamics Study*; **Manjesh K. Singh**, Patrick Ilg, Rosa M. Espinosa-Marzal, Nicholas D. Spencer and Martin Kröger; *Polymers* **2016**, 8 (7), 254
- *Polymer Brushes under Shear: Molecular Dynamics Simulations Compared to Experiments*; **Manjesh K. Singh**, Patrick Ilg, Rosa M. Espinosa-Marzal, Martin Kröger and Nicholas D. Spencer; *Langmuir* **2015**, 31 (16), 4978-4805.
- *Combined Modeling and Experimental Studies of Interacting Polymer Brushes under Shear*; **Manjesh K. Singh**, Patrick Ilg, Rosa M. Espinosa-Marzal, Martin Kröger and Nicholas D. Spencer; 5th World Tribology Congress, WTC 2013. Vol. 3 Politecnico di Torino (DIMEAS), 2014. p. 2440-2442.
- *Polymer Brush based Tribology*; **Manjesh K. Singh**; Book-chapter (*submitted*).
- *Glass Transition Temperature of Disentangled Polymer Melts: Single-chain-nanoparticles approach*; **Manjesh K. Singh**, Minghan Hu, Yu Cang, Hsiao-Ping Hsu, Heloise Therien-Aubin, Kaloian Koynov, George Fytas, Katharina Landfester and Kurt Kremer; (*submitted*).
- *To Precipitate or to Mix: Why do Elastin-like Polypeptides have Different Solvation Behaviors in Water-ethanol and -urea Mixtures?*; Yani Zhao, **Manjesh K. Singh**, Kurt Kremer, Debashish Mukherji and Robinson Cortes-Huerto; (*submitted*).

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## REFERENCES

- Prof. Dr. Kurt Kremer, Director, Polymer Theory Department, Max Planck Institute for Polymer Research, Mainz, Germany. Email: [kremer@mpip-mainz.mpg.de](mailto:kremer@mpip-mainz.mpg.de)
- Prof. Dr. Nicholas D. Spencer, Department of Materials, Swiss Federal Institute of Technology (ETH), Zurich Switzerland. Email: [nicholas.spencer@mat.ethz.ch](mailto:nicholas.spencer@mat.ethz.ch)
- Prof. Dr. Martin Kroege, Department of Materials, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland. Email: [mk@mat.ethz.ch](mailto:mk@mat.ethz.ch)
- Prof. Dr. Patrick Ilg, School of Mathematical and Physical Sciences, University of Reading, United Kingdom Email: [p.ilg@reading.ac.uk](mailto:p.ilg@reading.ac.uk)
- Prof. Dr. Rosa M. Espinosa Marzal, Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, United States. Email: [rosae@illinois.edu](mailto:rosae@illinois.edu)
- Prof. Dr. Vikram Jayaram, Divisional Chairman, Division of Mechanical Sciences, Indian Institute of Science, Bangalore, India. Email: [qjayaram@materials.iisc.ernet.in](mailto:qjayaram@materials.iisc.ernet.in)