

# CURRICULUM VITAE

Gaurav Prakash Shrivastav

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**Present Address:**

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**Date & Place of birth:** 25-FEB-1983, Allahabad, India.

**Marital Status:** Married

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## PROFESSIONAL EXPERIENCE

1. Postdoctoral fellow (March 2019 - present, in the group of Prof. Dr. Gerhard Kahl)  
Institute für Theoretische Physik  
Technische Universität Wien.  
Vienna, Austria.  
Project: Microscopic approaches to the nonlinear mechanics of driven defect-rich crystals.
2. Postdoctoral fellow (Jan 2017 - Feb 2019, in the group of Prof. Dr. Sabine H. L. Klapp)  
Institute für Theoretische Physik  
Technische Universität Berlin.  
Berlin, Germany.  
Project: Rheology of suspensions of liquid crystals and magnetic colloids.
3. Postdoctoral fellow (Jan 2013 - Dec 2016, in the group of Prof. Dr. Jürgen Horbach)  
Institute für Theoretische Physik II- Soft Matter,  
Heinrich-Heine-Universität Düsseldorf.  
Düsseldorf, Germany.  
Project: Rheology of glasses.

## RESEARCH INTERESTS

- **Mechanical properties of glass:** Yielding, shear bands, elastic moduli, residual stresses.
- **Mixtures of liquid crystals and magnetic colloids:** self-assembly, rheology, shear banding.
- **Spin systems with quenched disorder:** Random field Ising model (RFIM), ground-state morphology, phase transitions.
- **Mass transport models:** mass dependent fragmentation and aggregation, steady-state distributions.

## SPONSORED RESEARCH PROJECTS

1. *Origin of Residual Stresses in Metallic Glasses*  
**Project leader:** Dr. Gaurav Prakash Shrivastav  
**Mentor:** Prof. Dr. Jürgen Horbach  
**Date of Award:** November 2014  
**Funding Agency:** Deutsche Forschungsgemeinschaft (DFG), SPP 1594  
**Publication:** “Shear band relaxation in a deformed bulk metallic glass”, I Binkowski, **G. P. Shrivastav**, J. Horbach, S. V. Divinski, G. Wilde, Acta Mater. **109**, 330 (2016).

## MASTER STUDENTS CO-SUPERVISED

1. Student: Mehrdad Golkia (HHU Düsseldorf, 2014-2016)  
Project: Residual stresses in Glasses  
Publication: “*On the Poisson’s ratio of deformed Pd based Bulk Metallic Glasses*”, N. Nollmann, V. Hieronymus-Schmidt, H. Rösner, M. Golkia, **G. P. Shrivastav**, J. Horbach, G. Wilde, under review (2018).

## EDUCATION

**Ph.D:** Theoretical Physics (2006 - 13)  
Jawaharlal Nehru University, New Delhi, India.

**Thesis Title:** Aggregates and Interfaces in Nonequilibrium Systems

### Thesis Supervisors:

Prof. Dr. Sanjay Puri  
School of Physical Sciences  
Jawaharlal Nehru University  
New Delhi, India.

Prof. Dr. Varsha Banerjee  
Department of Physics  
Indian Institute of Technology Delhi  
Hauz-Khas, New Delhi, India.

**M.Sc.:** Physics (2003 - 05)  
Dr. Ram Manohar Lohiya Avadh University, Faizabad, India, % of marks: 66.80, Division: First

**B.Sc.:** Physics, Chemistry, Mathematics (2000 - 03)  
Ewing Christian College, University of Allahabad, India, % of marks: 59.83, Division: Second

## COMPUTER SKILLS

**Languages:** FORTRAN, C, C++, Python.

**Operating Systems:** Linux, Windows, Mac OS, adept in working on HPC clusters in SGE and SLURM environments.

**Softwares Packages:** LAMMPS, VASP, Graph-Cut, Mathematica, Matlab, MPI

**Simulation Techniques:** Molecular Dynamics, *ab initio* Molecular Dynamics, Monte Carlo, Combinatorial Optimization.

## LANGUAGES KNOWN

1. English : Fluent
2. German : Basic (A1.2)
3. Hindi : Native speaker

## PROFESSIONAL ACTIVITIES

1. Reviewed papers for Soft Matter, Journal of Rheology, Crystals, Phil. Magazine Letters and Applied Physics A.

## EXTRA-CURRICULAR ACTIVITIES

1. Convener, Journal Club, School of Physical Sciences, JNU (Jul 2008- Jul 2009).
2. System Administrator, Ph.D. Computational Lab, School of Physical Sciences, JNU (Nov. 2009-Jul 2010).

## ACADEMIC ACHIEVEMENTS

1. Recipient of **Gold Medal** in M.Sc.

2. Qualified National Eligibility Test for Lectureship **UGC- NET** in June 2006.
3. Won the **best poster award** in SPS March Meeting on Soft Matter Physics held on 04-05 March, 2010 at Jawaharlal Nehru University, New Delhi.
4. Won the **best poster award** in SPS@25 Looking Forward on 10-11 March, 2011 at Jawaharlal Nehru University, New Delhi.

## PUBLICATIONS

1. “Anomalous transport of magnetic colloids in a mixture of liquid crystals and magnetic colloids”, **G. P. Shrivastav**, S. H. L. Klapp, *Soft Matter* **15**, 973 (2019). (Impact factor: 3.709)
2. “Yielding of glass under shear: a directed percolation transition precedes shear-band formation”, **G. P. Shrivastav**, P. Chaudhuri, J. Horbach, *Phys. Rev. E* **94**, 042605 (2016). (Impact factor: 2.366)
3. “Heterogeneous dynamics during yielding of glasses: Effect of aging”, **G. P. Shrivastav**, P. Chaudhuri, J. Horbach, *J. Rheol.* **60**, 835 (2016). (Impact factor: 2.916)
4. “Shear band relaxation in a deformed bulk metallic glass”, I Binkowski, **G. P. Shrivastav**, J. Horbach, S. V. Divinski, G. Wilde, *Acta Mater.* **109**, 330 (2016). (Impact factor: 6.036)
5. “Non-Porod behavior in systems with rough morphologies”, **G. P. Shrivastav**, V. Banerjee, S. Puri, *Eur. Phys. J. E* **37**, 1 (2014). (Impact factor: 1.802)
6. “Ground-state morphologies in the random-field Ising model: Scaling properties and non-Porod behavior”, **G. P. Shrivastav**, M. Kumar, V. Banerjee, S. Puri, *Phys. Rev. E* **90**, 032140 (2014). (Impact factor: 2.366)
7. “Fractal Domain Morphologies: Signatures and Implications”, Varsha Banerjee, Sanjay Puri, **G. P. Shrivastav**, *Indian J. of Phys.* **88**, 1005 (2014). (Impact factor: 0.988)
8. “Scattering Properties of Paramagnetic Ground States in the Three-Dimensional Random-Field Ising Model”, **G. P. Shrivastav**, S. Krishnamoorthy, V. Banerjee, S. Puri, *Europhys. Lett.* **96**, 36003 (2011). (Impact factor: 1.834)
9. “Mass-transport models with multiple-chipping processes”, **G. P. Shrivastav**, V. Banerjee, S. Puri, *Eur. Phys. J. B* **78**, 217 (2010). (Impact factor: 1.536)
10. “Mass-transport models with fragmentation and aggregation”, **G. P. Shrivastav**, V. Banerjee, S. Puri, *Phase Transitions* **83**, 140 (2010). (Impact factor: 1.028)

## TEACHING ASSISTANTSHIPS

1. Teaching Assistant, Mathematical Physics,  
Course Instructor: Prof. Dr. Sanjay Puri, School of Physical Sciences, JNU New Delhi, (Monsoon Semester, 2008).
2. Teaching Assistant, Statistical Mechanics,  
Course Instructor: Prof. Dr. Brijesh Kumar, School of Physical Sciences, JNU New Delhi, (Winter Semester, 2009).
3. Teaching Assistant, Advanced Topics in Classical and Quantum Mechanics,  
Course Instructor: Prof. Dr. Akhilesh Pandey, School of Physical Sciences, JNU New Delhi, (Monsoon Semester, 2010).
4. Teaching Assistant, Statistical Mechanics,  
Course Instructor: Prof. Dr. Sanjay Puri, School of Physical Sciences, JNU New Delhi, (Winter Semester, 2010).
5. Teaching Assistant, Quantum Mechanics,  
Course Instructor: Prof. Dr. Jürgen Horbach, Institute für Theoretische Physik II- Soft Matter, HHU Düsseldorf, (Summer Semester, 2014).

6. Teaching Assistant, Computational Physics,  
Course Instructor: Prof. Dr. Jürgen Horbach, Institute für Theoretische Physik II- Soft Matter,  
HHU Düsseldorf, (Winter Semester, 2014/15).
  7. Teaching Assistant, Statistical Physics,  
Course Instructor: Prof. Dr. Reinhold Egger, Institute für Theoretische Physik IV, HHU  
Düsseldorf, (Winter Semester, 2015/16).
  8. Teaching Assistant, Mathematical Physics,  
Course Instructor: Prof. Dr. Hartmut Löwen, Institute für Theoretische Physik II- Soft Matter,  
HHU Düsseldorf, (Summer Semester, 2016).
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## REFERENCES

1. **Prof. Dr. Sanjay Puri**  
School of Physical Sciences,  
Jawaharlal Nehru University, New Delhi -110067.  
E-mail: puri@mail.jnu.ac.in
2. **Prof. Dr. Varsha Banerjee**  
Department of Physics,  
Indian Institute of Technology Delhi, New Delhi -110016.  
E-mail: varsha@physics.iitd.ac.in
3. **Prof. Dr. Jürgen Horbach**  
Institut für Theoretische Physik II - Soft Matter,  
Heinrich-Heine-Universität Düsseldorf,  
E-mail: horbach@thphy.uni-duesseldorf.de
4. **Prof. Dr. Sabine Klapp**  
Institut für Theoretische Physik  
Technische Universität Berlin  
E-mail: sabine.klapp@tu-berlin.de
5. **Prof. Dr. Pinaki Chaudhuri**  
The institute of Mathematical Sciences  
CIT Campus, Taramani, Chennai -600113.  
E-mail: pinakic@imsc.res.in

## SUMMARY OF RESEARCH

My research broadly focuses on computational statistical physics. The problems on which I am working are as follows:

### Dynamics and Rheology of mixtures of liquid crystals and magnetic colloids

Suspensions of magnetic colloids inside liquid crystalline matrix, have attracted much research attention in the past few decades. These systems show a rich variety of self-assembled structures and have a wide range of biomedical and technical applications. The equilibrium phases of magnetic colloids in the liquid crystal matrix are well studied via computer simulations. Experiments and Monte Carlo simulations have demonstrated that in the nematic phase liquid crystals impose nematic order in the magnetic colloids. However, the dynamics and rheology of these suspensions is not well understood.

To understand the effects of the relative sizes of the two species and the aspect ratio of liquid crystals on the dynamics and rheology of such mixtures, we study 80:20 binary mixture of liquid crystals and magnetic colloids. The interaction among liquid crystals are modeled by Gay-Berne potential while magnetic colloids interact via a soft sphere and a long ranged dipolar interactions. Liquid crystals and magnetic colloids both show isotropic to nematic phase transition as the density is increased.

We observe that in case where the sizes of the two components are comparable, liquid crystals display a diffusive behaviour at all densities in the isotropic phase. Magnetic colloids, on the other hand, remain subdiffusive in the isotropic phase. In the nematic phase, liquid crystals show diffusion in the direction parallel and perpendicular to the nematic director. Magnetic colloids show a diffusive behaviour parallel to the nematic director, while remain subdiffusive in the perpendicular direction.

We also study the rheology of above mixture by imposing a constant shear rate in the planer Couette geometry. Our initial results suggest that the mixture shows a shear thinning behaviour. Liquid crystals and the chains of magnetic colloids both align in the shear direction. The degree of alignment is higher in the magnetic colloids. The flow curve for the mixture shows a mild non-monotonic behaviour at low shear rates.

#### Publicatons:

1. “Anomalous transport of magnetic colloids in a mixture of liquid crystals and magnetic colloids”, **G. P. Shrivastav**, S. H. L. Klapp, *Soft Matter* **15**, 973 (2019).

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## Mechanical Properties of Glasses

The mechanical properties of amorphous solids have been extensively harnessed in recent years. However, a complete microscopic understanding of the mechanisms leading to macroscopic response of these materials is still missing. In order to develop materials with specific functions, it is necessary to have an improved knowledge of the underlying processes which lead to different macroscopic properties.

**Yielding of Glasses:** Glassy materials, ranging from soft matter systems to metallic alloys, yield under external mechanical loading. Yielding transition in glasses has been an area of intense research in recent years, especially the nature of this transition is highly debated. Using extensive molecular dynamics simulations, we identify the dynamical heterogeneities (regions with contrasting

mobilities) in glasses under imposed shear. At a critical strain, these highly mobile regions percolate and the material yields. We give evidence that this yielding transition belongs to the universality class of directed percolation. During yielding, these materials often respond via formation of inhomogeneous flow patterns (shear bands) which are precursors to the catastrophic failure. At low shear rates, the percolating cluster, formed at the onset of flow, evolves into a transient shear band. We also demonstrate that transient shearbands are visible only under specific combinations of age of glass sample, ambient temperature and imposed shear rate, signifying the dependence of material properties of glasses on the history of preparation.

**Publications:**

1. “*Yielding of glass under shear: a directed percolation transition precedes shear-band formation*”, **G. P. Shrivastav**, Pinaki Chaudhuri, Jürgen Horbach, Phys. Rev. E **94**, 042605, 2016.
2. “*Heterogeneous dynamics during yielding of glasses: effect of aging*”, **G. P. Shrivastav**, Pinaki Chaudhuri, Jürgen Horbach, J. Rheol. **60**, 835 (2016).

**Residual stresses in Glasses:** When a sheared glass is allowed to relax, stress does not decay to zero but tends towards a finite value and a new (deformed) glass state is obtained. We find that the amount of residual stress in glasses depends on the initial stress before the shear cessation. Also, its evolution is governed by the preshear rate. The spatially resolved mean square displacement of particles suggests that the residual stresses remain localized in regions where shear band has been present before. The deformed glass, obtained after shearing and relaxation, shows new mechanical properties. It has higher Poisson’s ratio, i.e. it is more plastic than the undeformed glass.

**Publications:**

1. “*Shear band relaxation in a deformed bulk metallic glass*”, I Binkowski, **G. P. Shrivastav**, J. Horbach, S. V. Divinski, G. Wilde, Acta Mater. **109**, 330 (2016).
2. “*On the Poisson’s ratio of deformed Pd based Bulk Metallic Glasses*”, V. Hieronymus-Schmidt, H. Rösner, M. Golkia, **G. P. Shrivastav**, J. Horbach, G. Wilde, under review in Acta Mater. (2018).

## Spin Systems with Quenched Disorder

Spin systems with quenched disorder have been one of the most researched topic in the last few decades. Though these systems are ubiquitous, the complex nature of the spin-spin interactions create difficulties in studying them theoretically and computationally.

**Ground-state morphology of random field Ising model:** In order to understand the effect of quenched disorder on spin systems, we consider the random field Ising model (RFIM), which is an archetypal example of magnetic systems with quenched disorder. In the RFIM, the behavior of the phases and phase transitions is still controversial. An issue of interest for these systems is regarding their thermodynamic ground state. At  $T = 0$ , all the information about the system is encoded in the ground state. Further, according to the *zero-temperature fixed point hypothesis*, transitions at  $T = 0$  and  $T \neq 0$  are in the same universality class. Therefore, a study of the ground-state morphology at  $T = 0$  is important in understanding the RFIM phase diagram. We characterize the ground state morphologies of RFIM at  $T = 0$  using a state-of-art graph-cut algorithm introduced by Boykov and Kolmogorov (BK). The literature on combinatorial optimization provides many graph-cut algorithms with different polynomial complexity times. This BK algorithm is faster (the polynomial time complexity  $\sim O(N)$ ) than any other and yields exact ground states. These ground states show novel morphological features which are analyzed by calculating spin-spin correlation functions and structure factors. The methodologies used in this study helped us to identify fractal

morphologies in diverse physical systems such as dilute anti-ferromagnets, binary fluid mixtures, stochastic growth phenomena, etc.

**Publications:**

1. “Scattering Properties of Paramagnetic Ground States in the Three-Dimensional Random-Field Ising Model”, **G. P. Shrivastav**, S. Krishnamoorthy, V. Banerjee, S. Puri, Europhys. Lett. **96**, 36003 (2011).
2. “Ground-state morphologies in the random-field Ising model: Scaling properties and non-Porod behavior”, **G. P. Shrivastav**, M. Kumar, V. Banerjee, S. Puri, Phys. Rev. E **90**, 032140 (2014).
3. “Non-Porod behavior in systems with rough morphologies”, **G. P. Shrivastav**, V. Banerjee, S. Puri, Eur. Phys. J. E **37**, 1 (2014).

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## Mass Transport Models

Mass transport models form a general class of lattice models defined by dynamics in which mass is transferred stochastically from site to site. These models have been used to study such diverse situations as traffic flow, clustering of buses, force propagation through granular media, surface growth, river networks etc. An important issue in these models is to understand the non-equilibrium steady states and the nature of phase transitions when different kinetic processes like fragmentation, aggregation, diffusion etc. are varied.

**Mass-independent fragmentation:** In many physical situations fragmentation of mass is independent of the mass of the fragmenting piece. In this context, we have studied a class of conserved mass-transport models in which the elementary move is the fragmentation and aggregation of chips of mass  $k$  with  $k = 1; 2; 3; 4; \dots$  etc. The steady-state probability distributions of these models, in mean field limit, are characterized by a  $k$ - exponentially decaying branched structure. The population of these  $k$ - branches in the initial condition remains conserved in the steady-state.

**Mass-dependent fragmentation:** In many physical systems, the fragmentation of mass depends upon the masses of the chip size and the fragmenting cluster. Few experiments on *Au* nanoparticles report distinct chipping kernels for small and large cluster. The steady-state distribution in these systems are either exponentials or power laws or their combinations. In this regard, we have focused on the class of models which has mass-dependent diffusion term  $a(n)m^{-\alpha}$ , where  $n$  is the mass on a lattice site under consideration and  $m$  is the mass of the piece which is fragmenting from this site. We have used our results of multiple chipping processes to show that the steady-state probability distributions of these models are combination of many exponentially decaying functions.

**Publications:**

1. “Mass-transport models with fragmentation and aggregation”, **G. P. Shrivastav**, V. Banerjee, S. Puri, Phase Transitions **83**, 140 (2010).
2. “Mass-transport models with multiple-chipping processes”, **G. P. Shrivastav**, V. Banerjee, S. Puri, Eur. Phys. J. B **78**, 217 (2010).