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Jan 2010	Jan 2015	Graduate Student, Chemistry and Physics of Materials Unit, JNCASR, Bangalore, India.
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Research Topic

My research focuses on understanding the mechanical behavior of polymers under external stress, using computer simulations. Primary objective of the research is to elucidate the various phenomena governing the mechanical properties of polymer materials. One of the major objective this research is to develop force field parameters, which allows bond-dissociation phenomena during the molecular dynamics simulations.

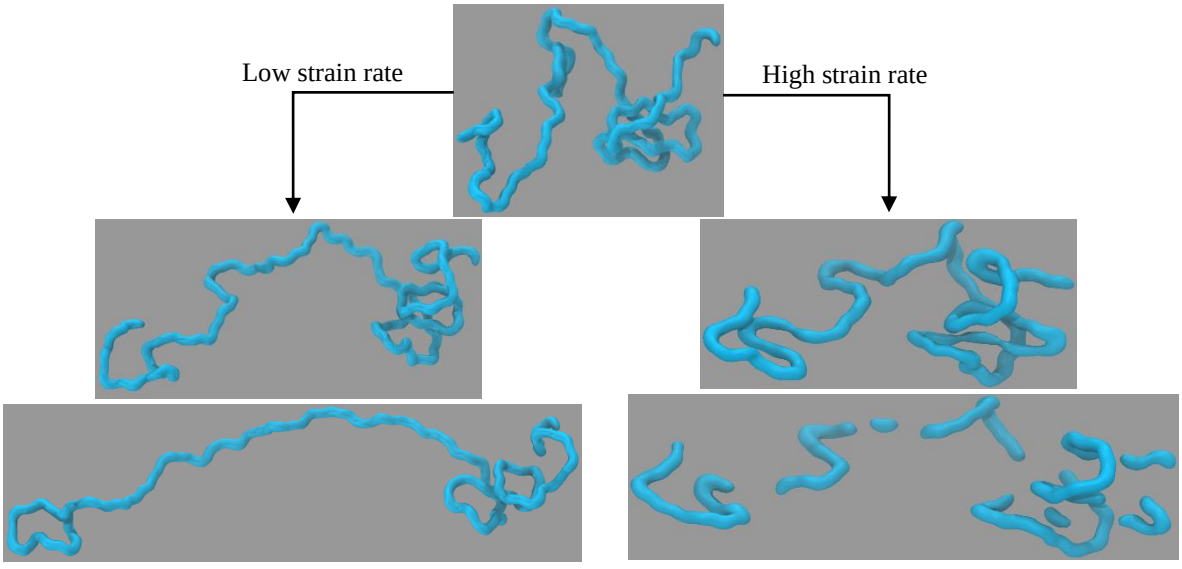

Figure: Behavior of polymer chain under the uniaxial tension.

Publications

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2. **R. S. Payal** and S. Balasubramanian, Dissolution of cellulose in ionic liquid: an ab-initio study, Phys. Chem. Chem. Phys., 2014, 16, 17458.

3. **R. S. Payal** and S. Balasubramanian, Effect of cation symmetry on organization of ionic liquids near a charged mica surface, J. Phys.: Condens. Mater., 2014, 26, 284101.

4. **R. S. Payal** and S. Balasubramanian, Homogeneous mixing of ionic liquids: molecular dynamics simulation, Phys. Chem. Chem. Phys., 2013, 15, 21077.

5. **R. S. Payal**, S. Balasubramanian, I. Rudra, K. Tandon, I. Mahlke, D. Doyle and R. Cracknell, Shear viscosity of linear alkanes through molecular simulations: quantitative test for n-decane and n-hexadecane, Mol. Sim., 2012, 38, 1234.

6. **R. S. Payal** and S. Balasubramanian, Dynamic atomics force microscopy for ionic liquids: massless model shows way, ChemPhysChem, 2012, 13, 3085.

7. **R. S. Payal** and S. Balasubramanian, Orientational ordering of ionic liquids near a charged mica surface, ChemPhysChem, 2012, 13, 1764

8. **R. S. Payal**, R. Bharath, G. Periyasami and S. Balasubramanian, Density functional theory investigation on structure and dissolution mechanism for cellobiose and xylan in an ionic liquid: gas phase and cluster calculations, J. Phys. Chem. B, 2011, 116, 833.

9. J. P. Singh, **R. S. Payal**, R. C. Srivastava, H. M. Agrawal, P. Chand, A. Tripathi and R. P. Tripathi,Effect of thermal treatment on the magnetic properties of nanostructured zinc ferrite, J. Phys. Conf. Ser., 2010, 217, 012108.