Poly-Nang-Big

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Our Group

- 1. Multiscale: Scaling from molecular interactions to large scale processes
- 2. Areas related with polymers &/or nano-science &/or biological applications
- 3. Fundamental understanding to application detailing
- 4. Combining experiments, theory and simulations
- 5. Inquisitiveness, Inspiration and Involvement





Indian Bratilation of Technology Implement Analyze Test Develop Conceive

- 39 Journal Publications
- 20+ Years of Experience
- 10+ Years in Industrial R&D
- Projects Worth ~175 lakhs (ongoing)

Activities: Hovering around Polymers



DBT Project (Collaboration with LVPEi; Ongoing): Multiple-Drug Nano-formulation and Quantitative Imaging of Cellular Response for Glaucoma Treatment Protocol

Internal Collaborator: Dr. Lopamudra Giri

Objective Project Objectives

Objective 1



Role of PNB Group: Nano-Formulation

Debasmita, JRF

of Hydrogels for Controlled Release

External Collaborators

Dr. Subhabrata Chakrabarti Dr. Sirisha Senthil Dr. Indrjeet Kaur



Normal vision





Fabrication of hydrogel based eye drop with multidrug nano-formulations using bioadhesive and thermosensitive polymer

Objective 2

Development of quantitative imaging tool to monitor drug release profile and measurement of intracellular calcium (cytosolic calcium) and cell viability by scanning laser confocal microscopy

Objective 3



Polypropylene: Controlled Branching



Scientific & Technological Content

- First validated mechanistic kinetic model for PP long chain branching
- Optimal variable space and meta-modeling to control polymer architecture in PP
- Isotactic backbones and atactic side chains by binary iron (metallocene) and zirconium single-site catalysts
- Catalyst (1) => Short chain atactic polypropylene macromonomers (aPP; having terminal double bonds)
- Catalyst (2) => Copolymerize isotactic propylene with aPP to form LCB PP

Grafting Density => Long chain branching formation rate w.r.to propagation rate



Kinetic scheme for the two catalyst systems.

- Initiation $C_1 + M \stackrel{k_{il}}{\longrightarrow} P_1$
- Propagation
- $P_n + M \xrightarrow{k_{\mathrm{p1}}} P_{n+1}$
- β -H elimination $P_n \xrightarrow{k_\beta} D_n^= + C_1^{\text{H}}$
- Reversible chain transfer to metal $D_n^{=} + C_1^{\mathrm{H}} \stackrel{K_{\mathrm{Br}}}{\longrightarrow} P_n$
- Reinitiation $C_1^{\text{H}} + M \stackrel{k_{\text{ri1}}}{\longrightarrow} P_1$

- Catalyst activation $\operatorname{cat}_2 + \operatorname{cocat} \stackrel{k_{a2}}{\to} C_2$
- Initiation
- $C_2 + M \xrightarrow{k_{i2}} Q_{1,0}$
- Propagation
 - $Q_{n,i} + M \stackrel{k_{\rm p2}}{\to} Q_{n+1,i}$
- Long chain branching
 Q_{n,i} + D⁼_{m,0} ^{αk_{lcb}}→ Q_{n+m,i+1}
 Chain transfer to costal
- Chain transfer to coctalyst
- $Q_{n,i} + \operatorname{cocat} \xrightarrow{k_{\mathrm{al}}} R_{n,i} + C_2^{\mathrm{Me}}$
- Reinitiation
- $C_2^{\text{Me}} + M \stackrel{k_{\text{ral}}}{\to} Q_{1,0}$
- Biomolecular deactivation $2Q_{n,i} \xrightarrow{k_{d_2}} 2R_{n,i} + 2C_d$

Chemical Engg. Journal, 2014 Poly. Engg. & Sci., 2014



Dr. K Mitra, IITH (Collaborator)



Dr. Anitha

Alkane Chains & Others: Interfacial Tension (Dissipative Particle Dynamics - DPD)





Collaborative Ongoing Project with Tata Steel: Utilization of Tailing Coal



Lignin Depolymerization



Linkage Type	Softwood (%)	Hardwood (%)
β–O–4 Aryl Ether	46	60
α−O−4 Aryl Ether	6-8	6-8
4-0-5 Diaryl Ether	3.5-4	6.5
β–5–phenylcoumaran	9-12	6
5-5-Biphenyl	9.5-11	4.5
β-1-(1,2-Diarylpropane)	7	7
$\beta-\beta-(Resinol)$	2	3
Others	13	15

Flexible



Major Highlights:

Catalyst: HZSM-5 Co-catalyst: NaOH Mild Reaction Conditions High Lignin Loading (12g)



G-Protein Diffusion: Molecular Simulation (Coarse Graining)



Approach to Fabricate Nanofiber based Novel Drug Carrier





Soya nuggets – A Potential Carrier: Release of Hydrophobic Drugs



Cardamom Shell: Low Cost Cross-linker Free Drug Carrier with High Loading



Piperine as Placebo: Sustained Release





Contact angle measurements (a) Gelatin Film (b) Gelatin/Naproxen Film (c) Gelatin/Piperine (20mg/ml) (d) Gelatin/Piperine (10 mg/ml) (e) Gelatin/Piperine (5 mg/ml) (f) Gelatin/Piperine (2.5 mg/ml)

Fundamental Studies on Ionic Polymers (PE)



Gelatin in a Coulombic Soup of Monovalent Salt (Molecular Dynamics)



Research Prospects



Few M.Tech Students





Deepak & Prasanna, 2015

Deepa, 2016

Rucha, 2017

Tithi, 2019





Remembering Contributions

Current Research Scholars













- Project worth ~175 Lakhs (ongoing) •
- GYTI-2016 Award (Student) ٠









May we all be protected May we all be nourished May we work together with great energy May our intellect be sharpened Let there be no animosity amongst us Peace (in me), peace (in nature), peace (in divine forces) - Upanishad

