Computational Studies of Soft Materials: Linking Molecular Level Features to Macroscopic Structure and Thermodynamics

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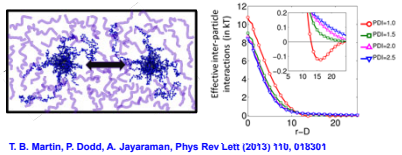
Polymer Functionalized Nanoparticles in Solutions and in Composites

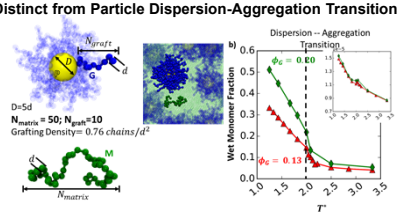
Using a combination of Polymer Reference Interaction Site Model (PRISM) theory and molecular simulations (Monte Carlo as well as molecular dynamics) we examine how the design of the polymer functionalized or grafted on the nanoparticle impacts the nanoparticle dispersion/assembly in a polymer matrix (or blend). These computational results are then compared directly to experimental scattering results obtained in our collaborator's labs.

Polydisperse Graft Polymers Improve Particle Dispersion in Matrix Polymers



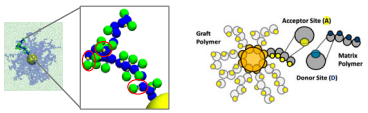
T. B. Martin, P. Dodd, A. Jayaraman, Phys Rev Lett (2013) 110, 018301

Graft-Matrix Polymer Wetting-Dewetting Transition Distinct from Particle Dispersion-Aggregation Transition



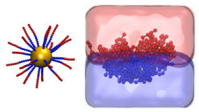
T. B. Martin, A. Jayaraman et al., JACS (2015) 137, (33), 10624
T. B. Martin, A. Jayaraman, Macromolecules (2016) 49, (24), 9684

Impact of Attractive Hydrogen Bonding Interactions on Graft–Matrix Wetting and Free Volume



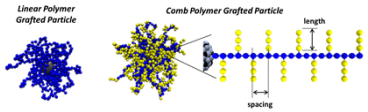
A. Kulshreshtha and A. Jayaraman, *Macromolecules* (2019) 52 (7), 2725-2735

Copolymer Grafted Nanoparticles Compatibilizing Interfaces in Homopolymer Blends



C.Estridge, A. Jayaraman ACS, Macro Letters (2015) 4, (2), 155

Branched versus Linear Graft Polymers



K. Modica, T. B. Martin, A. Jayaraman, Macromolecules (2017) 50, (12), 4854

REVIEW articles on this topic:

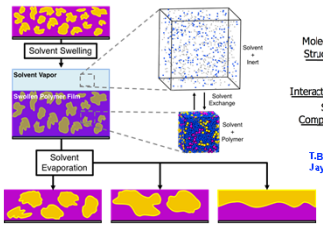
A. Jayaraman, J. Polymer Science B Poly. Phys. (2013) 51, (12), 524

V. Ganesan*, A. Jayaraman*, Soft matter (2014) 10, 13

Structure and Thermodynamics in Polymer-Solvent Mixtures

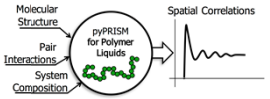
Using a combination of Polymer Reference Interaction Site Model (PRISM theory) and molecular simulations we predict how the interplay of solvent(s), polymer architecture and chemistry leads to novel assemblies as well as interesting previously unseen thermodynamics.

Simulation Method to Mimic Solvent Vapor Annealing



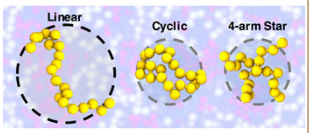
T.E. Gartner, III, T.H. Epps, III, A. Jayaraman, J. Chem. Theory Comput. (2016) 12, (11), 5501

Python Based Open Source Code for PRISM Theory (pyPRISM)



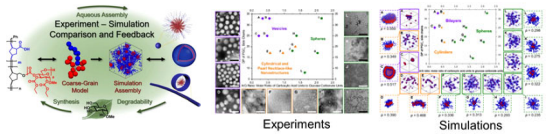
T.B. Martin, T.E. Gartner, III, R.L. Jones, C.R. Snyder, A. Jayaraman, Macromolecules (in review)

Linear, Cyclic, Star Homopolymers in Solvents

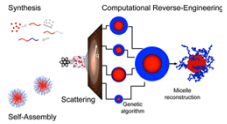


T.E. Gartner, III, A. Jayaraman, Soft Matter (2018) 14, 411

Assembly in Solutions of Amphiphilic Linear and Bottle Brush Copolymers



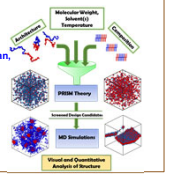
M. Dong, M. G. Wessels, J. Young Lee,..., D. Pochan, A. Jayaraman, K. Wooley *ACS Nano* (2019) 13, 5147-5162



D. J. Beltran-Villegas, M. G. Wessels, J. Young Lee, Y. Song, K. L. Wooley, D. J. Pochan, and A. Jayaraman, JACS (2019) 141 (37), 14916-14930

I. Lyubimov, M. Wessels, A. Jayaraman, *Macromolecules*, 2018, 51 (19), 7586

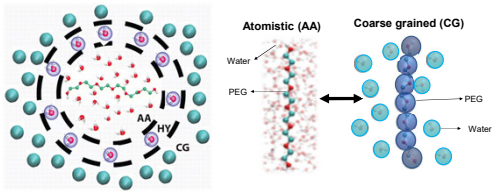
I. Lyubimov, D. J. Beltran-Villegas, A. Jayaraman, *Macromolecules*, 2017, 50, 7419



Bioinspired/Biomimetic Polymer Systems

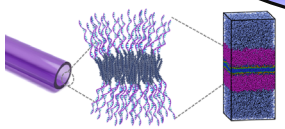
Using a combination of atomistic and coarse-grained molecular simulations we link molecular level features of nucleic acids and peptides containing materials to their macroscale interactions and structure.

Hybrid Atomistic – Coarse Grained Simulations



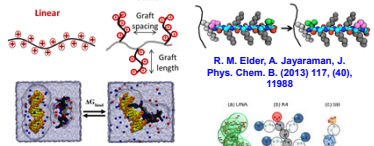
F.Stanzione, A. Jayaraman, J. Phys Chem B. (2016) 120, 4160

Self-Assembly of ssDNA Amphiphiles



H. Kuang, T.E. Gartner, III, A. Jayaraman, E. Kokkoli, ACS Appl. Nano Mater. (in review)

Design of Polycations for DNA Delivery



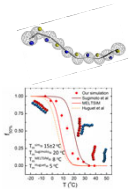
R. Elder, T. Emrick, A. Jayaraman, Biomacromolecules (2011) 12, (11), 3870

R. M. Elder, A. Jayaraman, J. Phys. Chem. B. (2013) 117, (40), 11988

A. Ghobadi, R. Letteri, T. Emrick, A.Jayaraman, Biomacromolecules (2016) 17, (2), 546

Thermoresponsive Polymers: Oligonucleic Acids, Elastin-Like Peptide, Collagen-Like Peptide

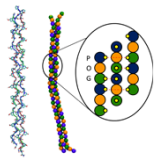
Our newly developed coarse-grained model to predict melting temperatures for oligonucleic acids with varying design (base sequence, backbone charge and flexibility)



A. Ghobadi , A. Jayaraman, Soft Matter (2016) 12, 2276

J. E. Condon, A. Jayaraman, Soft Matter (2017) 13, 6770

New coarse-grained model to predict melting temperatures for Collagen Like Peptide (CLP) triple helices



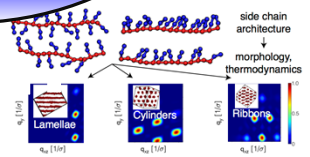
J. E. Condon , A. Jayaraman, J. Phys.Chem. B. (2018) in press

J. E. Condon#, T. B. Martin#, A. Jayaraman, Soft Matter (2017) 13, 2907

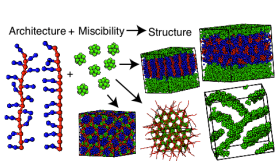
Optical and Photovoltaic Materials

Using coarse-grained simulations we a) predict the design of conducting polymers (electron donor) and fullerene derivatives (electron acceptor) to achieve a blend morphology that is optimal for high organic photovoltaic device efficiency and b) study how melanin chemistry and assembly techniques impact assembled nano- and microstructure for desired optical response of the materials.

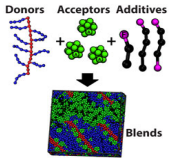
Design of Conjugated Polymer and Fullerene Derivatives for Organic Photovoltaic Materials



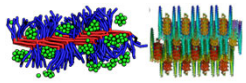
H. Marsh*, E. Jankowski*, A. Jayaraman, Macromolecules (2014) 47, (8), 2736



E. Jankowski*, H. Marsh*, A. Jayaraman, Macromolecules (2013) 46, (14), 5775



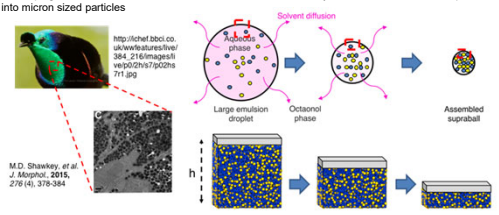
H. Marsh , A. Jayaraman, J. Polymer Science: Polymer Physics (2015) 53, (15), 1046



L. Zhang, F. Liu, Y. Diao, H.S. Marsh, N.S. Colella, A. Jayaraman, T.P. Russell, S.C.B. Mannsfeld, A. L. Briseno, JACS (2014) 136, (52), 18120

Melanin Nanoparticle Self-Assembly to Tailor Materials with Desired Color and Optical Response

Developing simulation methods to mimic reverse emulsion assembly of melanin and silica nanoparticles into micron sized particles



M.D. Shawkey, *et al. J. Morphol.*, **2015**, *276* (4), 378-384

Understanding structure within melanin nanoparticle as function of melanin chemistry and chain structure