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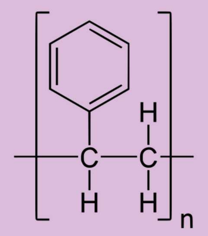
Simulations of Polymer-Grafted Nanoparticle Phase Behavior

Motivation

Composites of polymers and nanoparticles aim to form materials that combine the desirable mechanical, electrical, magnetic or other properties from each component.

Successful property combination depends on the overall morphology of the system and the polymer brush grafted to the the nanoparticle. The phase behavior, as a function of graft length, nanoparticle size and solvent, is a promising equilibrium control on morphology.

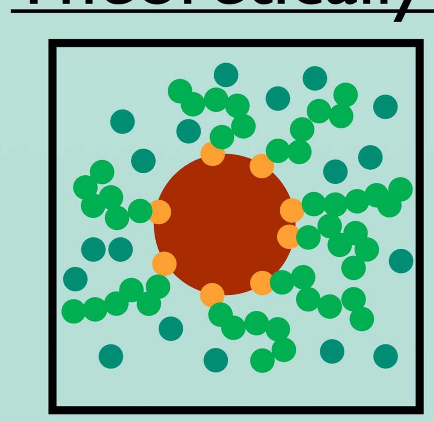
System†

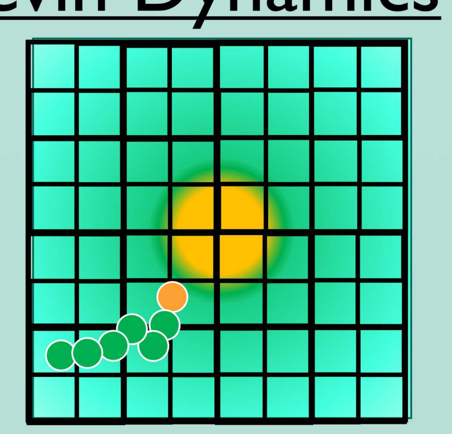


Au

System property	Experimental	TILD simulations
NP radius	10, 6 nm	7.47, 4.48 b
Graft mol. weight	21.5, 26.8, 31.4, 53 kDa	51, 63,74, 126 beads
Grafting density	1.01-0.59 or 0.1 chains/nm²	1.8-1.1 or 0.18 chains/b²

Theoretically-Inspired Langevin Dynamics (TILD) ‡





Particle-to-mesh scheme

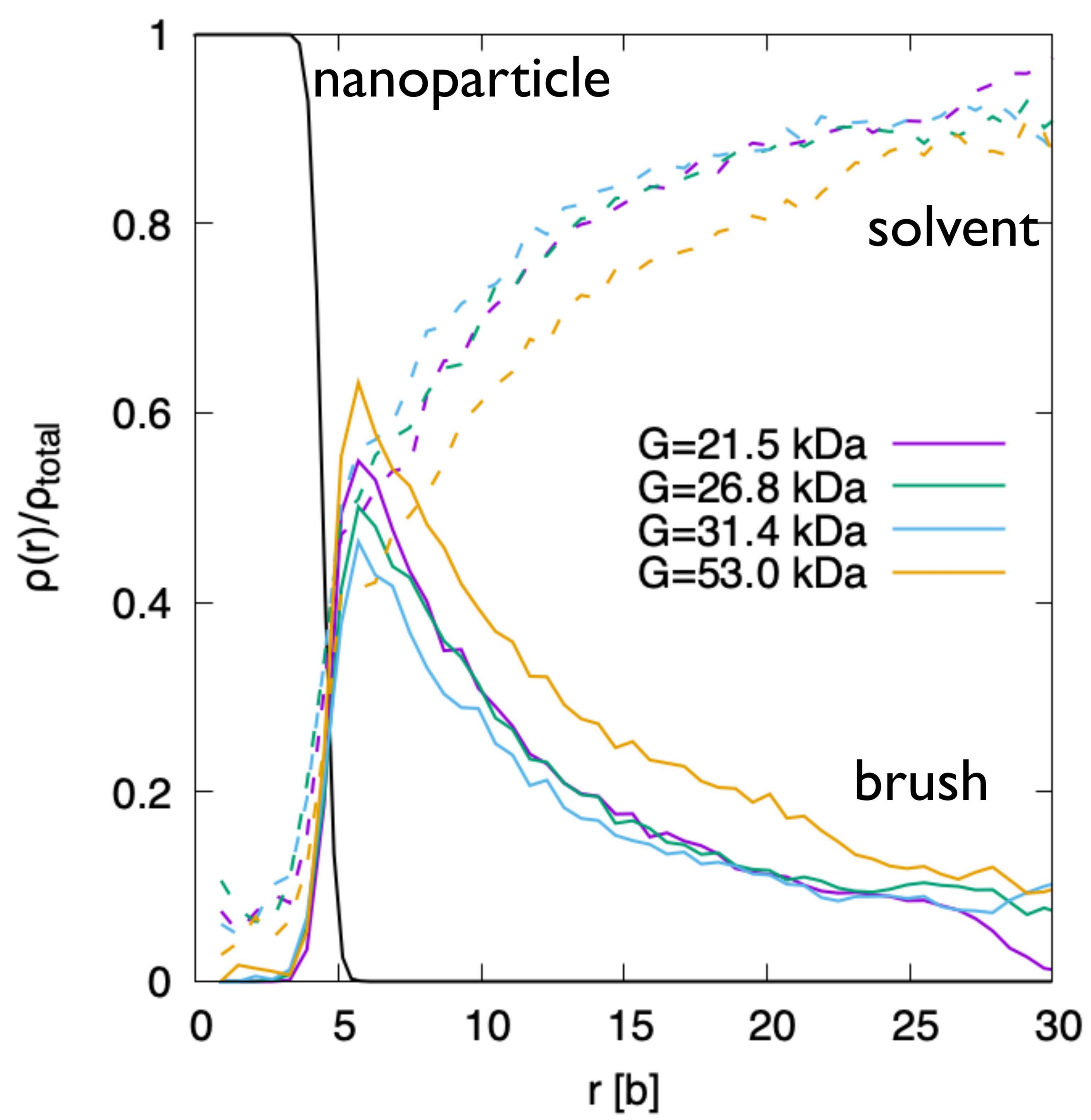
Procedure

- Molecular Dynamics evolves simulation of soft, point-based particles
- *T* is controlled with Langevin thermostat
- Force on particle is calculated from a field-based interaction

Benefits and losses

- Fast for particle-based method
- Takes of advantage of previous MD developments
- Thermal fluctuations
- No easy accesses to free energy

Brush profile



Brush profile (R_{NP}=6nm, χ=0.25)

Discussion

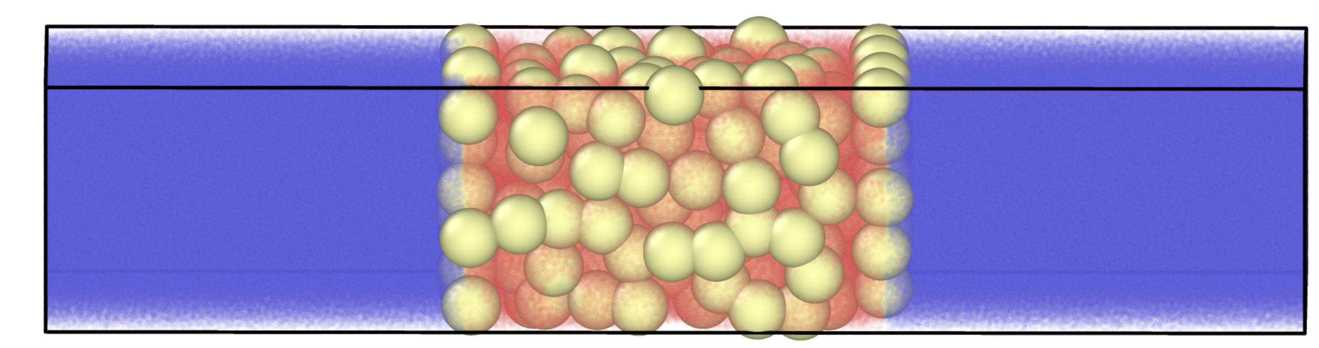
- Our method equilibrates long polymers in tractable times
- Phase separation can be induced by:
  1. Increasing polymer-nanoparticle interaction
  2. Increasing grafted polymer length
  3. Decreasing nanoparticle size

References

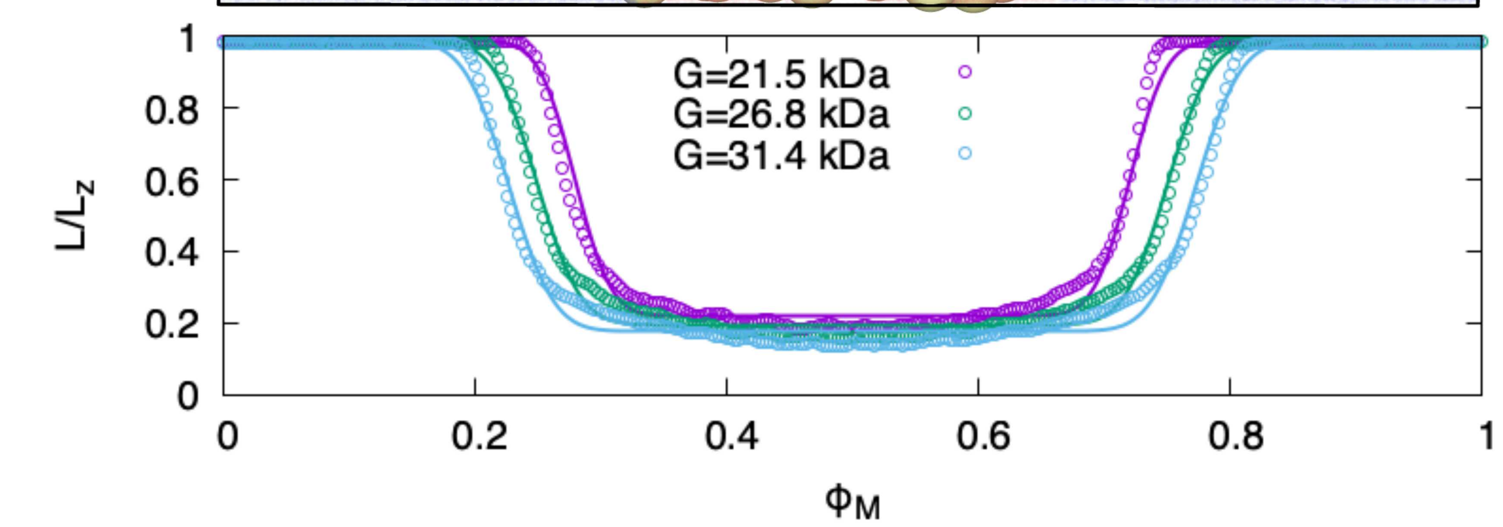
†Based on experimental system from Vaia *et al.*, Air Force Research Lab

‡Chao, H., Koski, J., & Riggleman, R.A. (2017). *Soft Matter*, *13*(1), 239–249.

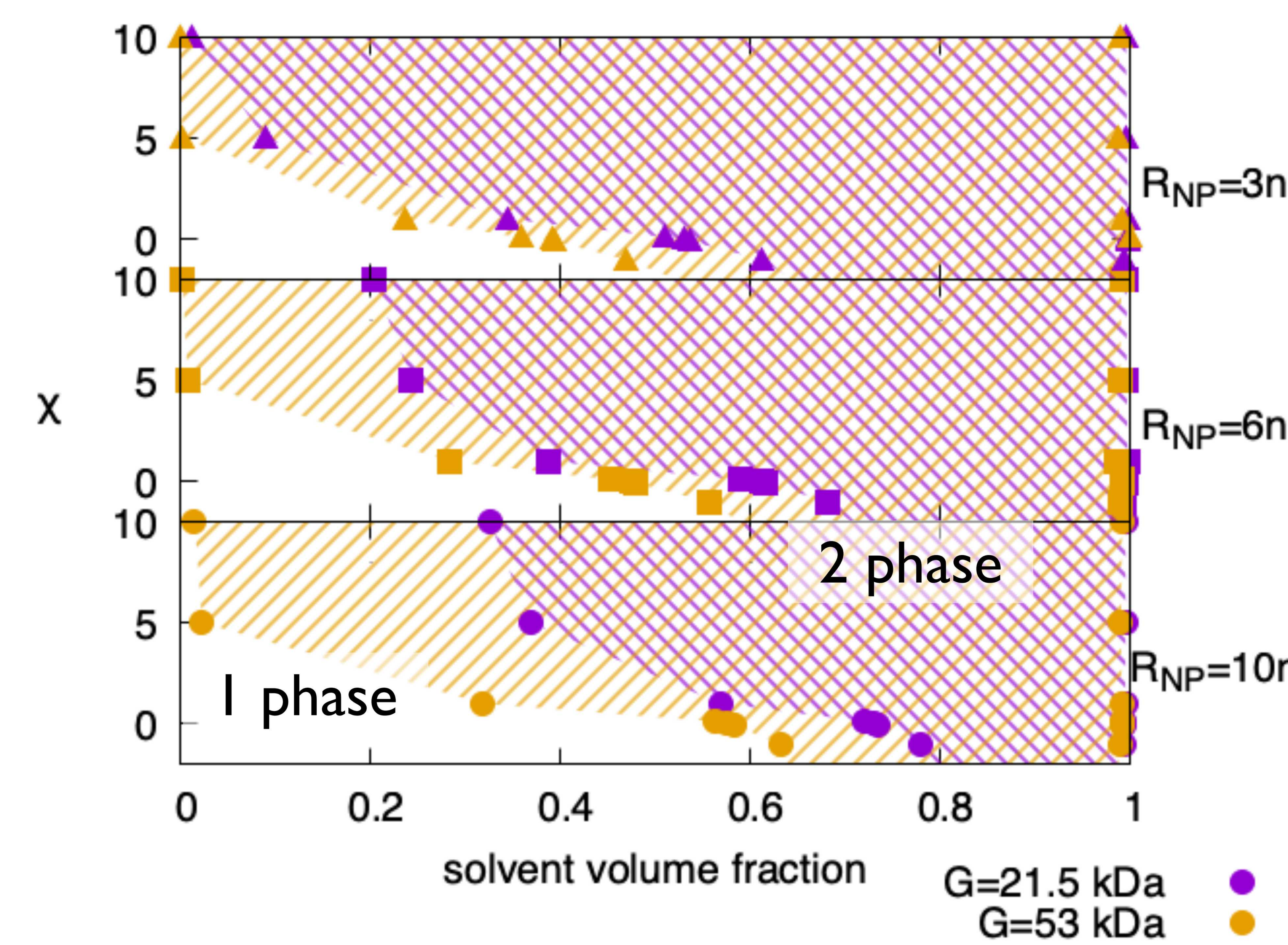
Phase behavior



Ex. config.



Density profile for different graft length (R_{NP}=3, χ=0)



Interaction parameter—vol. fraction phase diagram $\chi(\varphi)$

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