# Self-Assembly of Functional Nanoparticles

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# Functional nanoparticles

- building units of any ordered structures with tailored-in interactions through specific sites, ligand-particle interactions or amphiphilicity → many-body interactions

- ordered nanostructures → functional structures

- controlled synthesis (size, shape, ligand exchange rxns.)

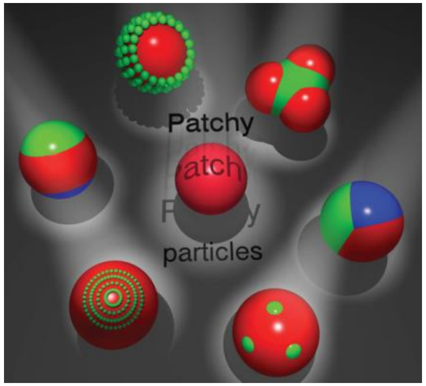
  fabrication

  consequences of assembly on properties

  application

# from anisotropic to isotropic units

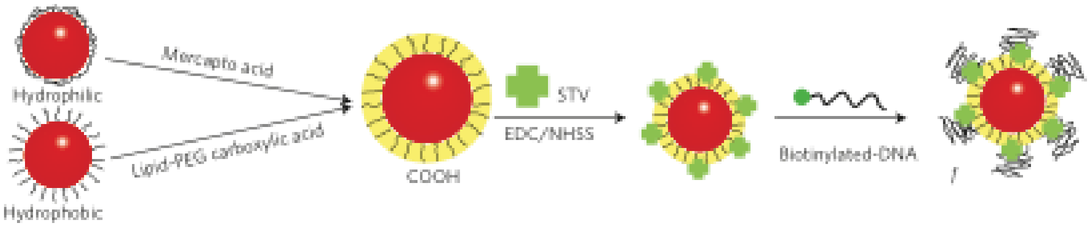
## Directed assembly




Kretzschmar, I., Macromol. Rapid Commun. 2010

Janus particles (supraparticular assembly; electric and magnetic fields)
- scaling, large volume production
-- limited to micron-size colloids
--- limited applications in sensors, phoretic motors

## Programmable assembly

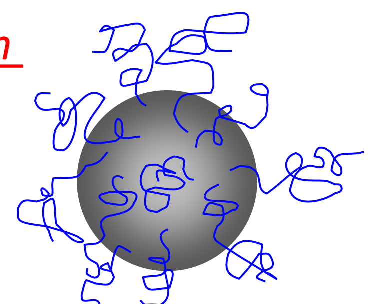


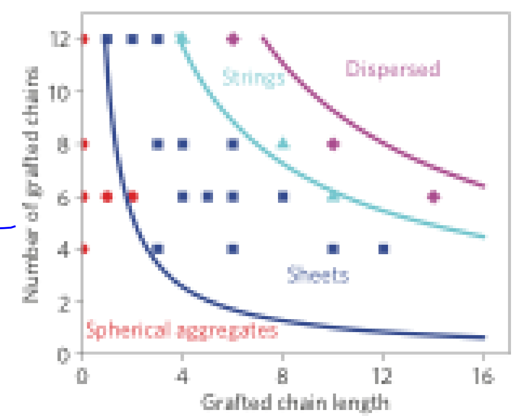

Gang, O., Nature Nanotechnology. 8, 865, 2013

- limited manufacturing
-- limited application of DNA-func. NPs
optical, field responsive properties
--- particle shape in binary heterolattices
heterogeneous systems

## Surfactant-like nanoparticles – Amphiphilicity in polymer-grafted NPs

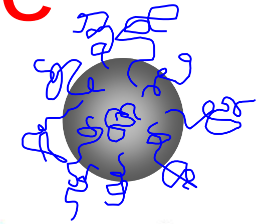
- well-controlled ligand attachments,
particle size and monodispersity
-- polymer nanocomposites beyond
mechanical properties

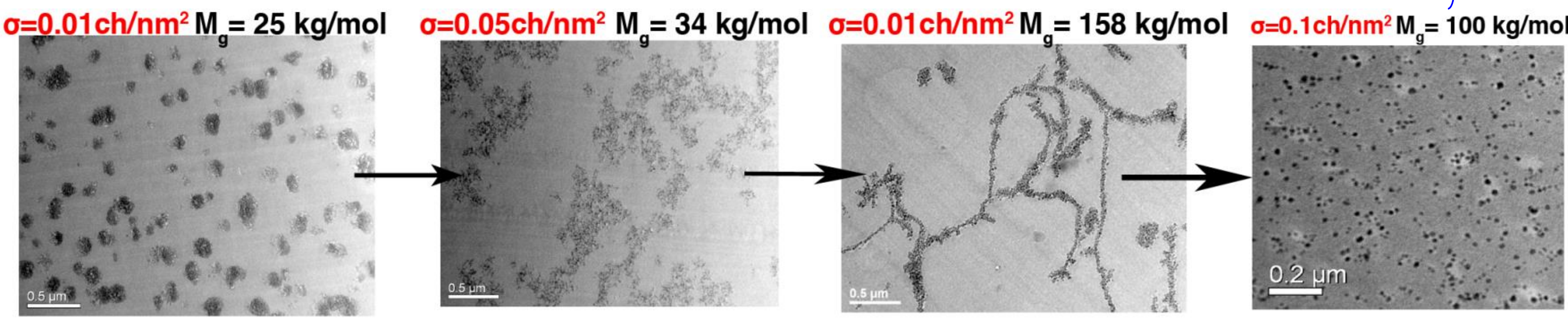





Akcora, P., Nature Materials. 8, 354, 2009

# Amphiphilic nanoparticles are like surfactants

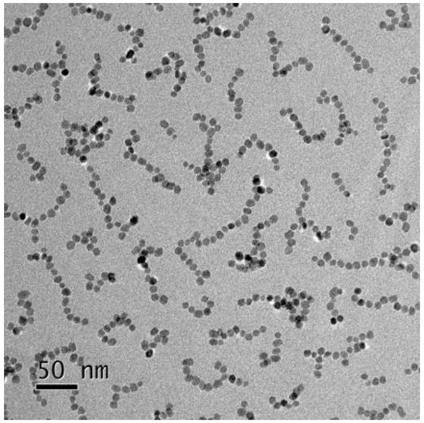




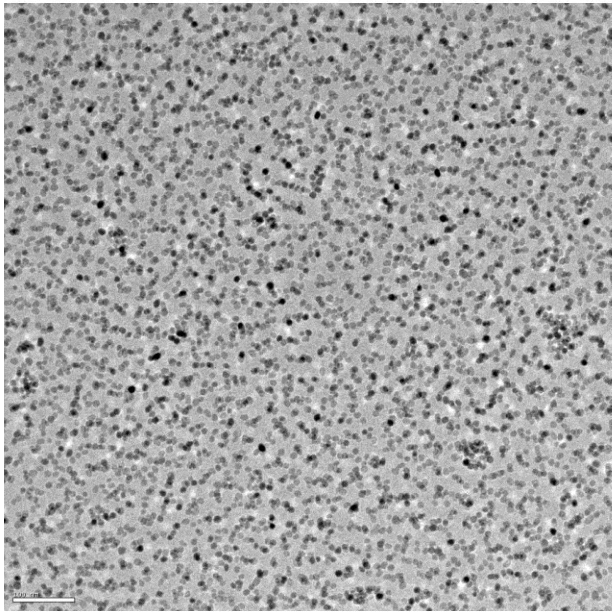

Akcora, P., Nature Materials. 8, 354, 2009

**anisotropy from isotropy**

- long grafts, low graft density, bimodal particle size tilt the energy landscapes to assemble particles in composites




strings of long-grafts of NPs in solution

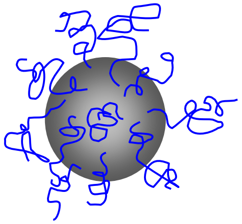


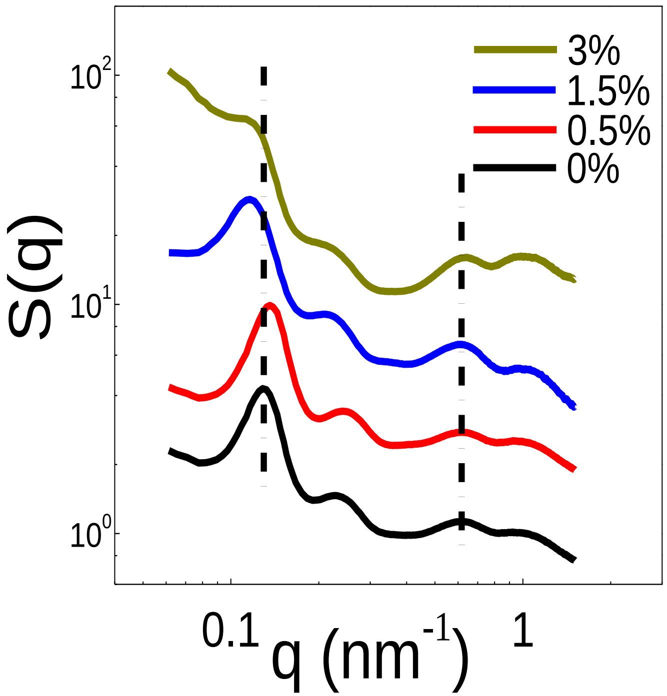
Scale bar: 100 nm

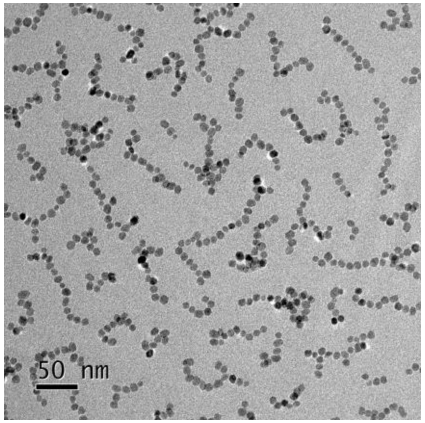
in bulk composite

Akcora, P., Macromolecules. 45, 3463, 2013
Akcora, P., Macromolecules. 47, 2030, 2014

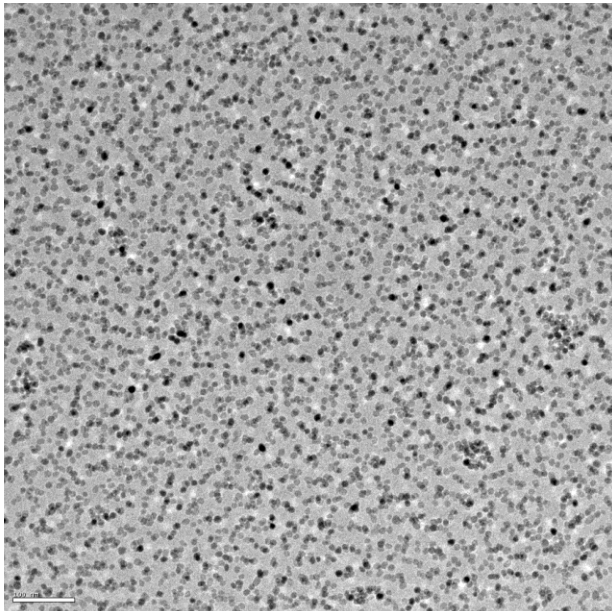
# Polymer-grafted nanoparticles are like surfactants






strings of long-grafts of NPs in solution



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in bulk composite


Macromolecules. 45, 3463, 2013
Macromolecules. 47, 2030, 2014

# Non-equilibrium effects

- filler aggregation
- external fields

} time and length scales in computer simulations do not overlap with experimental regimes

Unique structures in polymer nanocomposite (PNCs) → *e.g.* long-range repulsion and short-range attractions → theoretical models and computational frameworks are needed to study non-equilibrium effects

How can we quantify structure/function relationship that will correlate to system dynamics and mechanics (*e.g.* dynamical response of matrix chains) ?

Answer: By simpler material designs governed by well-controlled effective particle-particle interactions which can be simulated to understand non-equilibrium effects and mechanics under external fields.

→ material design for theory and experiments to work on real-problems and applications

# Polymer nanocomposites (PNCs)

- assembly of nanoparticles into 3-D structures
- interface and interphase effects in bulk composites
- understanding interfaces using rheology
- tailoring mesoscale properties of aggregates
- reversible assembly (mechanical responses under shear, fields)

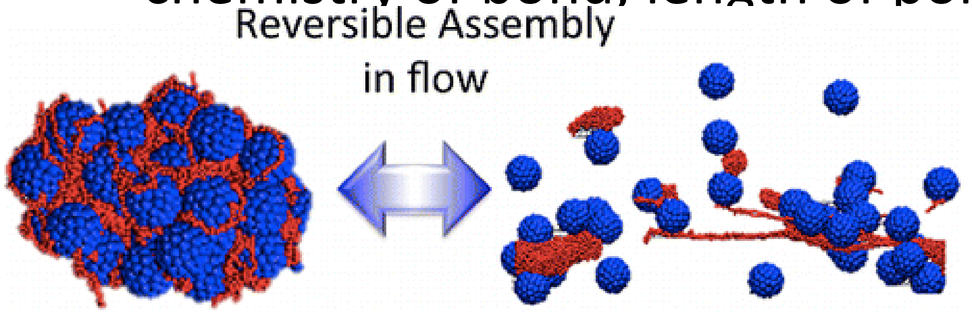
# ionic aggregation, assembly & transport

- ionic aggregation in homopolymers, BCs
- conducting polymers from assembled functional particle superstructures
- ion transport within confined spaces and assemblies

# Reversible assembly in flow

Dynamic self-assembly → ability to respond to changes in environment e.g. self-healing materials, targeted drug delivery

- Reversible polymer-colloid aggregates formed in shear flow
- Mechanical responses of systems controlled by flow, chemistry of bond, length of polymers




blood-clotting inspired reversible polymer-colloid composite assembly

adaptive behavior is based on different dissipation modes

Alexander-Katz, Nature Communication. 4, 2013; Macromolecules. 47, 2014

- *Bio-inspired self-assembly*: Building larger structures from small units