

Computational modeling & design of soft matter for engineering applications

Thomas M. Truskett

Graduate student recruiting weekend 2015



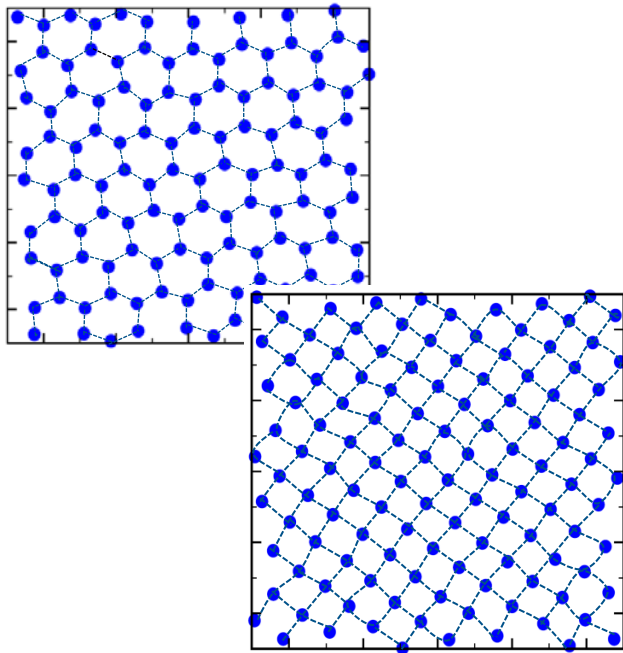
THE UNIVERSITY OF TEXAS AT AUSTIN

McKetta Department of
Chemical Engineering

Research projects

Inverse design of self-assembling nanocrystalline materials: From superlattices to reconfigurable mesoscopic networks

collaborations w/ Korgel & Milliron (National Science Foundation)



Jain et al. *Soft Matter* 9, 3866 - 3870 (2013)

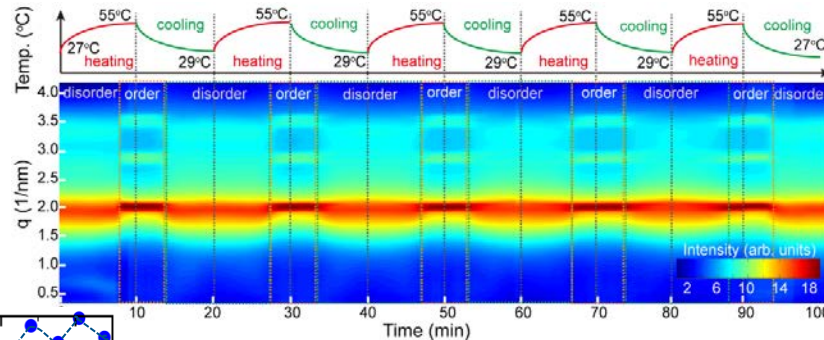
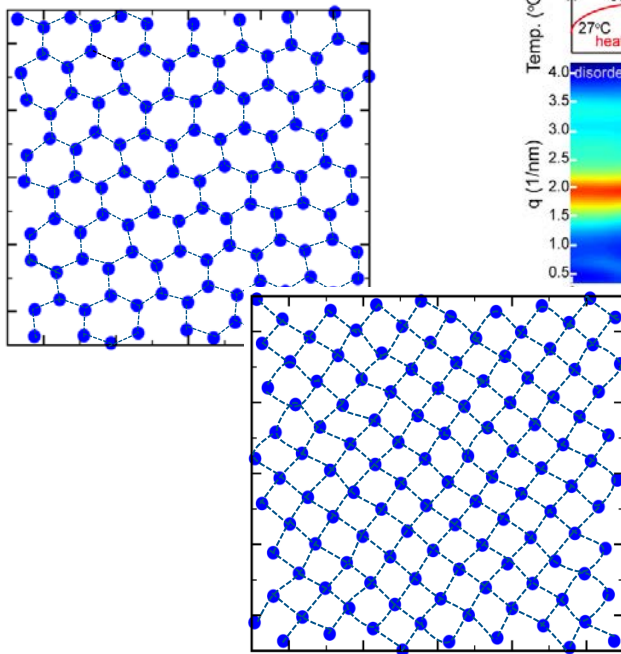
Jain et al. *J. Chem. Phys.* 139, 14112 (2013)

Jain et al. *Phys. Rev. X* 4, 031049 (2014)

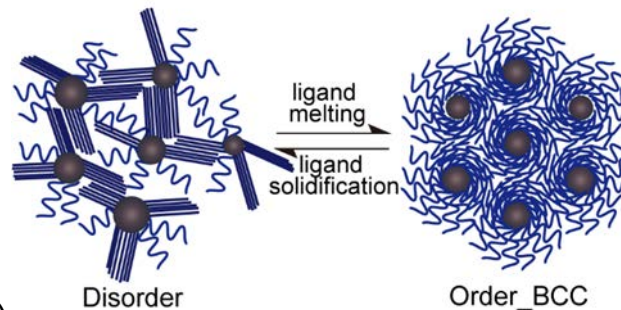
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Yu et al. *Faraday Discussions* (2015)



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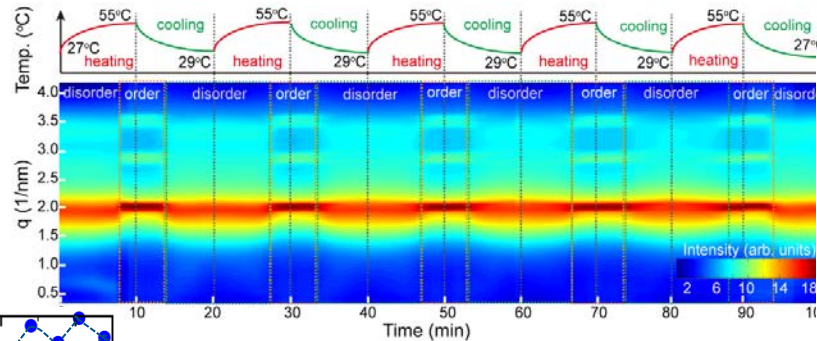
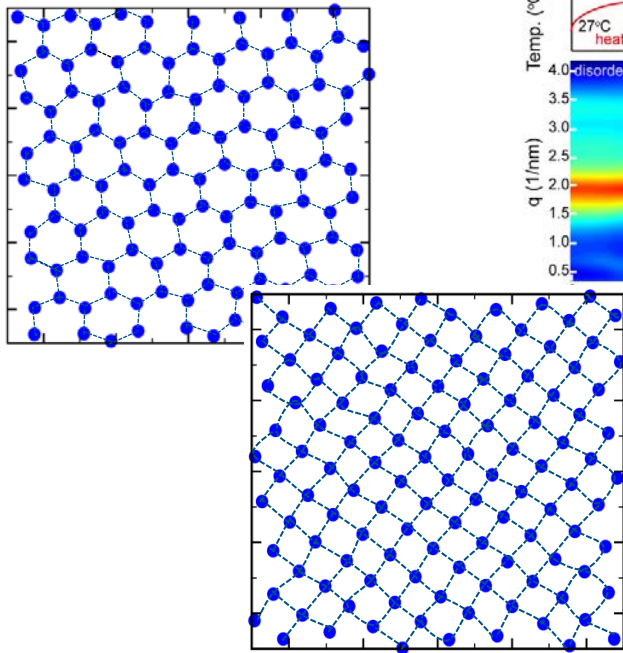
Jain et al. *J. Chem. Phys.* 139, 14112 (2013)

Jain et al. *Phys. Rev. X* 4, 031049 (2014)

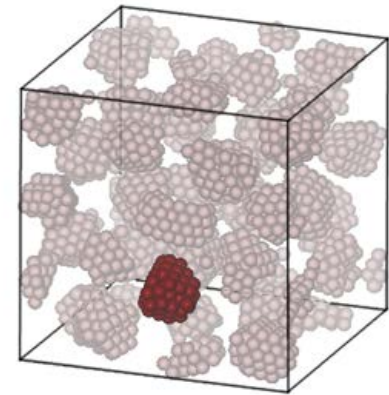
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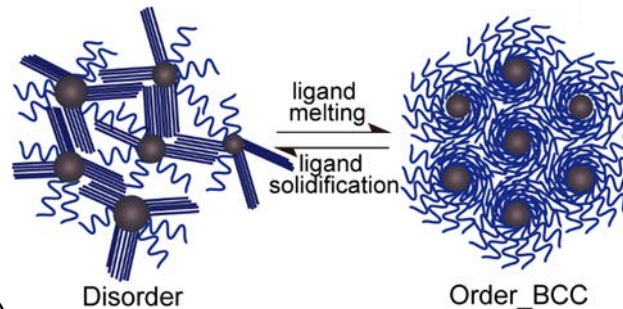
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Yu et al. *Faraday Discussions* (2015)



Jadrich et al.
Phys. Rev. Lett.
(under review)



Jain et al. *Soft Matter* 9, 3866 - 3870 (2013)

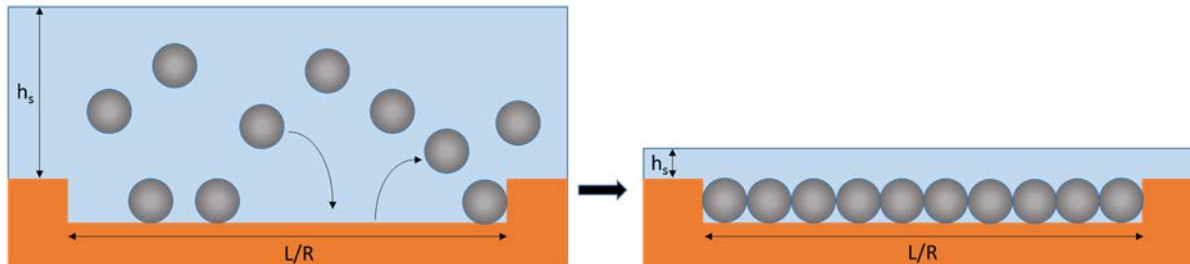
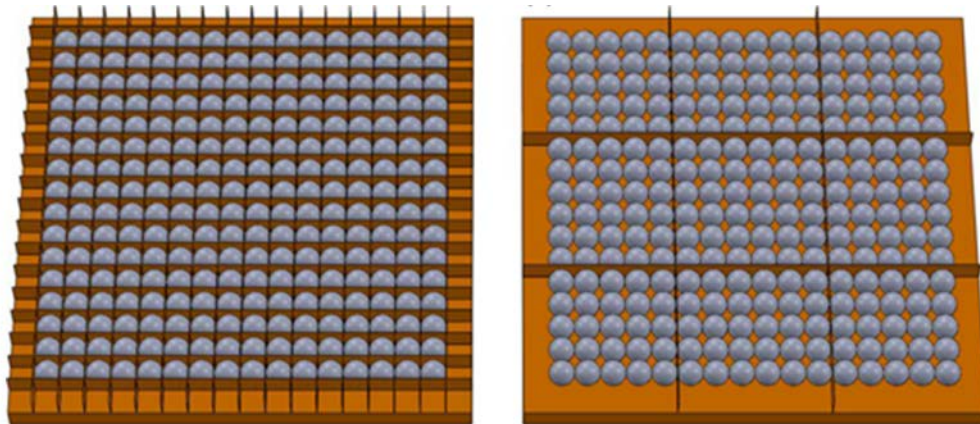
Jain et al. *J. Chem. Phys.* 139, 14112 (2013)

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Research projects

Graphoepitaxy for directed nanoparticle assembly

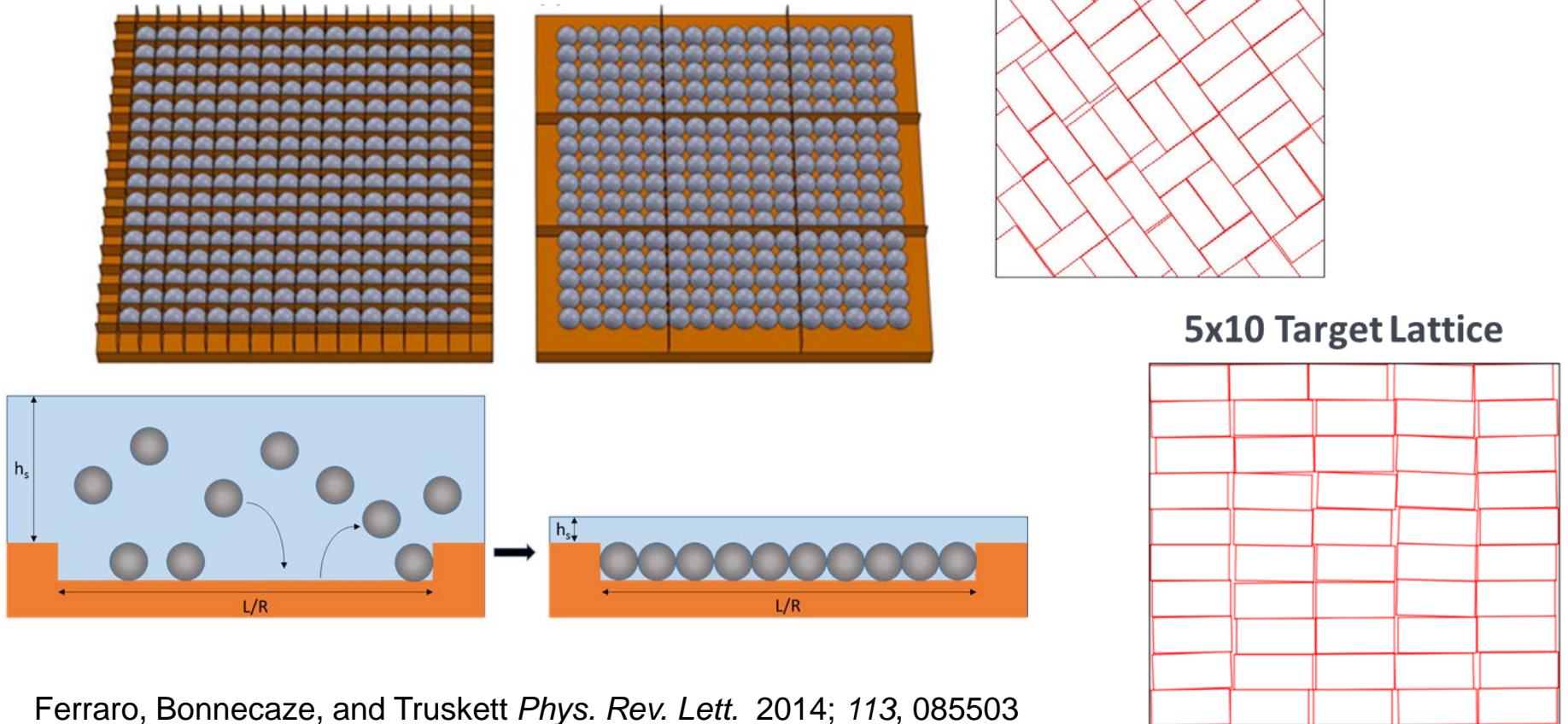
collaboration w/ Bonnecaze (NASA)



Research projects

Graphoepitaxy for directed nanoparticle assembly

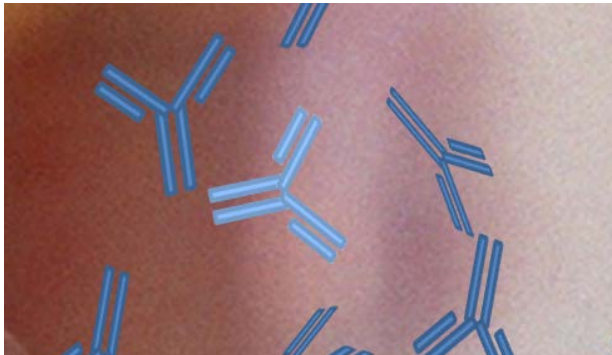
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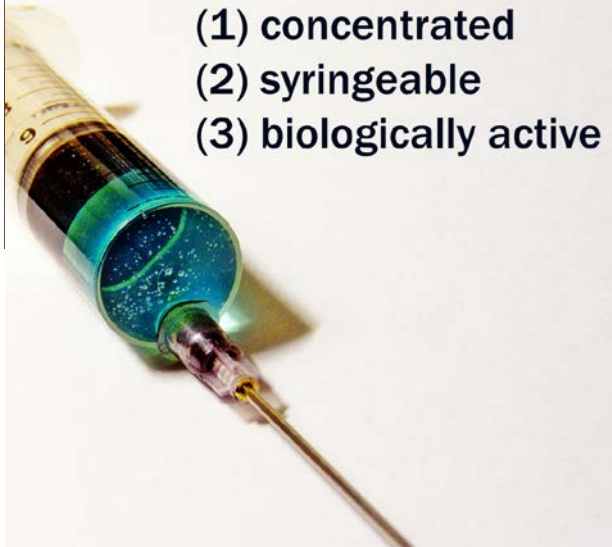
Research projects

Concentrated protein solutions for sub-Q injection

collaboration w/ Johnston & Maynard (NIH, NSF, industry)



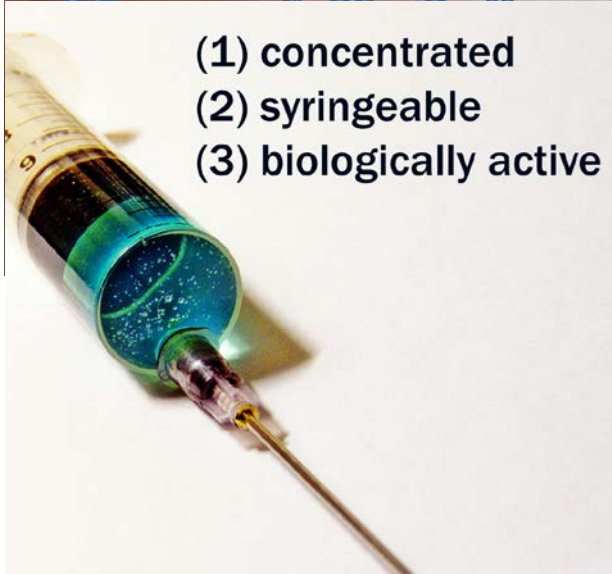
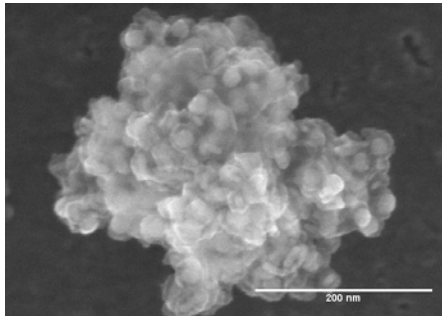
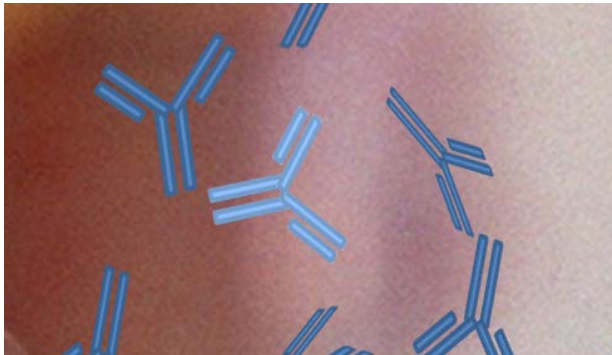
- (1) concentrated**
- (2) syringeable**
- (3) biologically active**



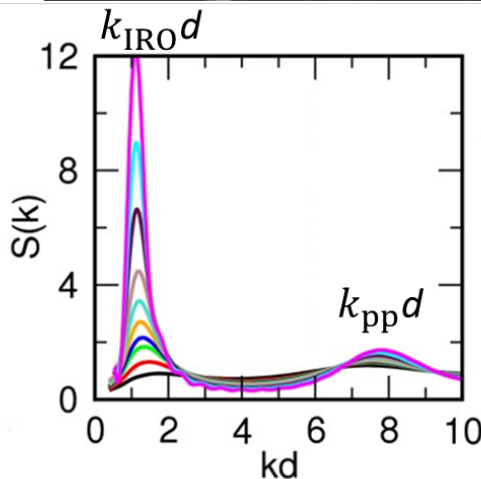
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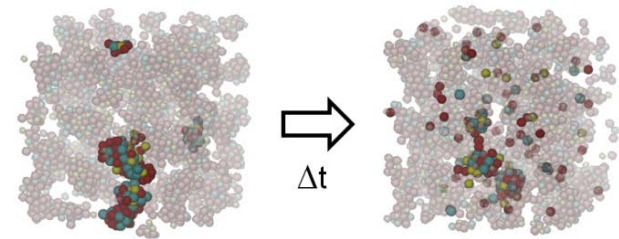
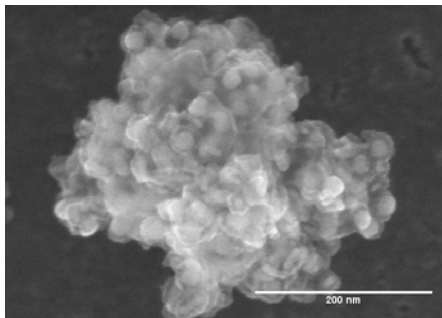
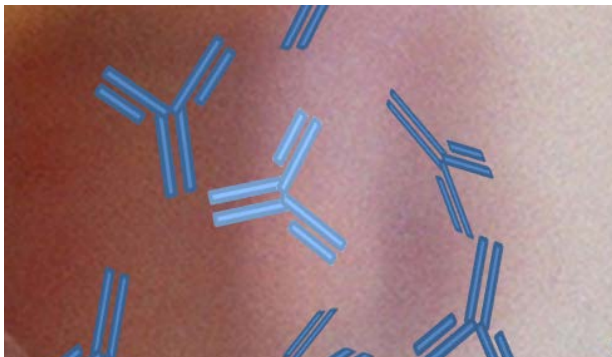


Johnston et al., *ACS Nano* (2012);
Borwankar et al. *Soft Matter* (2013)

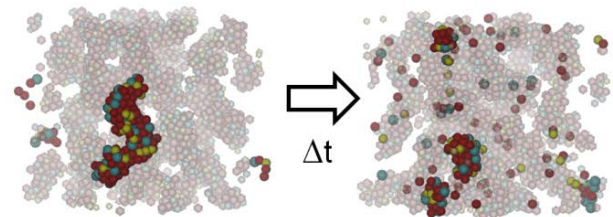
Research projects

Concentrated protein solutions for sub-Q injection

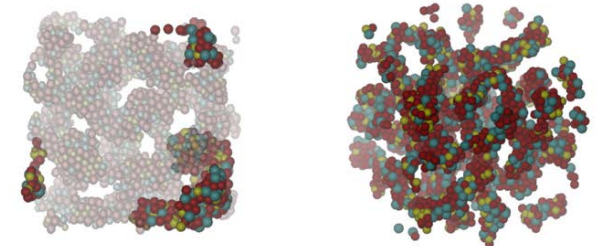
collaboration w/ Johnston & Maynard (NIH, NSF, industry)



(a) $\phi=0.125, \beta\epsilon=5.50$

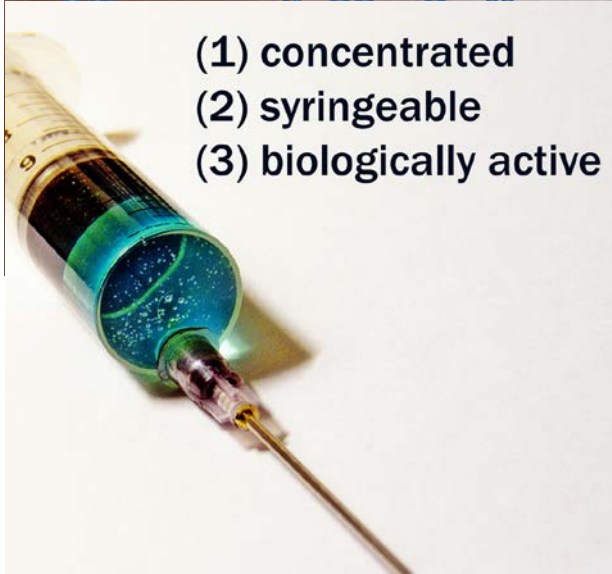


(b) $\phi=0.125, \beta\epsilon=5.80$

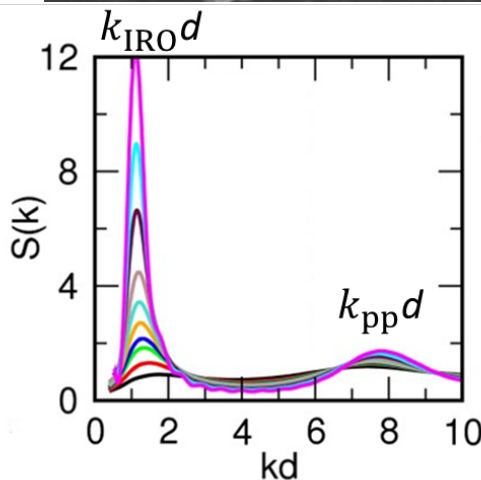


(c) $\phi=0.125, \beta\epsilon=6.30$

(d) $\phi=0.125, \beta\epsilon=6.80$



- (1) concentrated
- (2) syringeable
- (3) biologically active



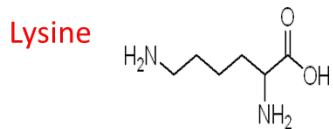
Johnston et al., *ACS Nano* (2012);
Borwankar et al. *Soft Matter* (2013)

Research projects

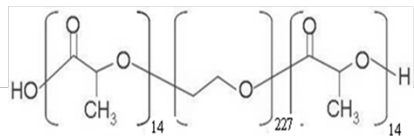
Assembling biodissociating gold nanoclusters for diagnostics and therapy

collaboration w/ Johnston and Sokolov (MD Anderson) (NIH)

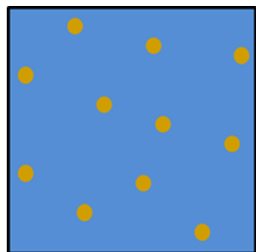
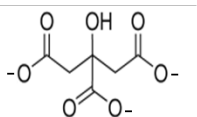
Murthy et al., *JACS* (2013); *ACS Nano* (2013);
J. Phys. Chem. C (2014)



PLA(1k)-PEG(10k)-PLA(1k)
Biodegradable

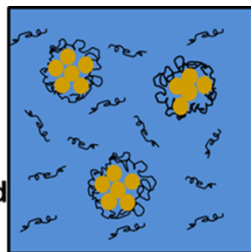


Citrate



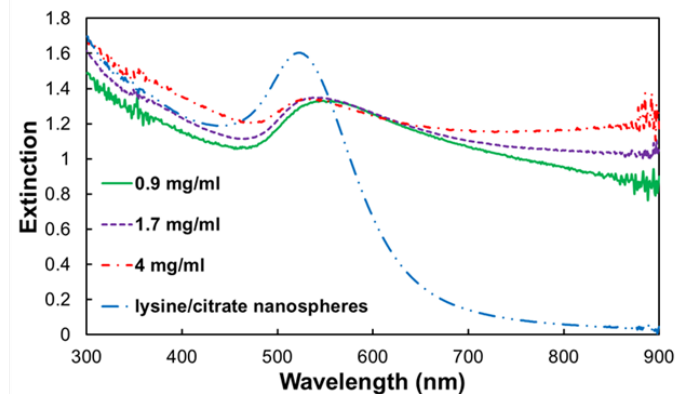
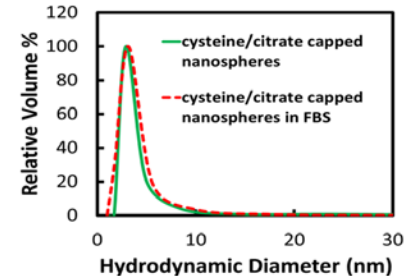
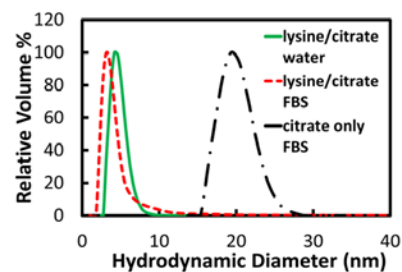
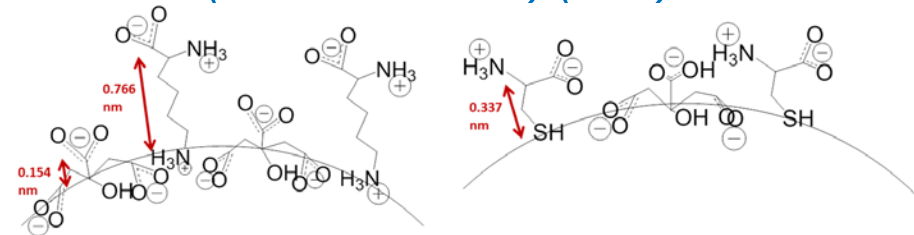
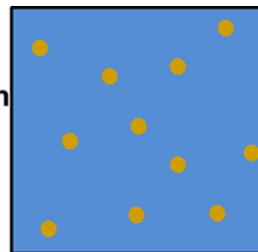
Polymer
Addition
Gold
Concentrated

pH 7



Polymer
Degradation

pH 5



Core skill set you can develop



- **Computational statistical mechanics**

Equilibrium and nonequilibrium molecular dynamics, Brownian dynamics, and Monte Carlo simulations. Stochastic optimization

Core skill set you can develop



- **Computational statistical mechanics**

Equilibrium and nonequilibrium molecular dynamics, Brownian dynamics, and Monte Carlo simulations. Stochastic optimization

- **Theory & Modeling**

Classical density functional theory , generalized Smoluchowski approaches, perturbation methods, integral equation theory, and coarse-graining strategies

Core skill set you can develop



- **Computational statistical mechanics**

Equilibrium and nonequilibrium molecular dynamics, Brownian dynamics, and Monte Carlo simulations. Stochastic optimization

- **Theory & Modeling**

Classical density functional theory , generalized Smoluchowski approaches, perturbation methods, integral equation theory, and coarse-graining strategies

- **Experimental characterization**

Static and dynamic light scattering, neutron scattering, and cryo-EM

QUESTIONS?

truskett@che.utexas.edu