Model Credibility and Model Reusability

Modeling Approach

Experimental Approach

Biomaterial Design

- Predictive assessments
- Reduce trial-and-error approach

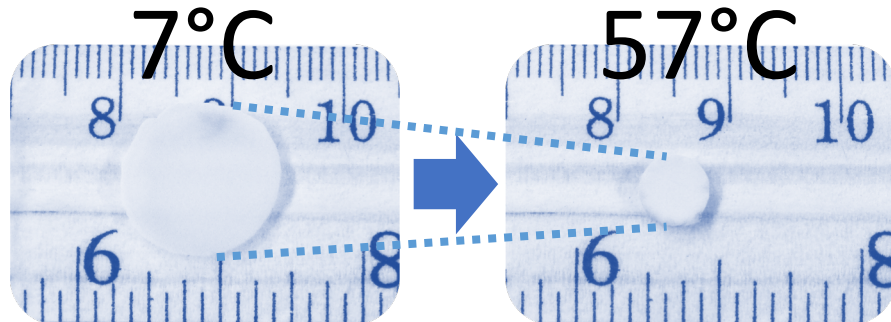**Markus Buehler** (MIT)

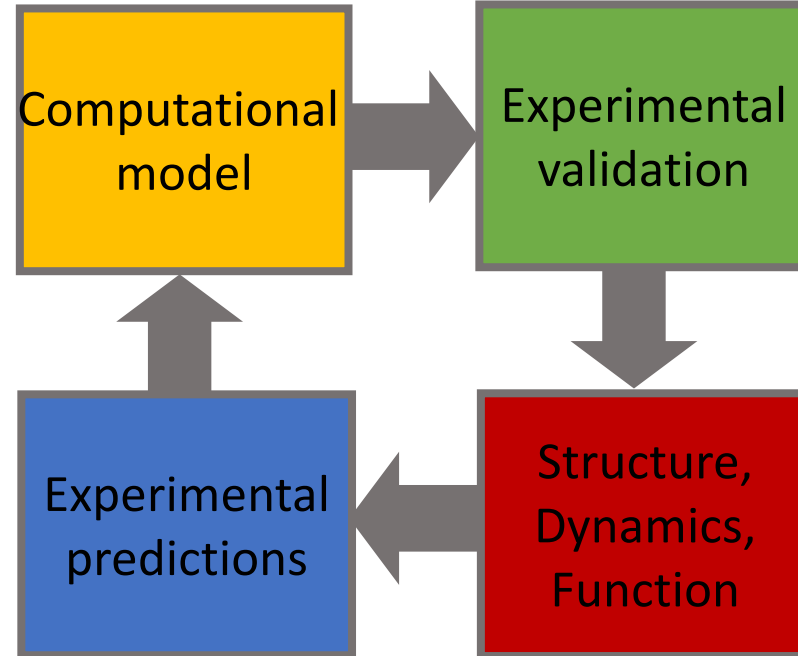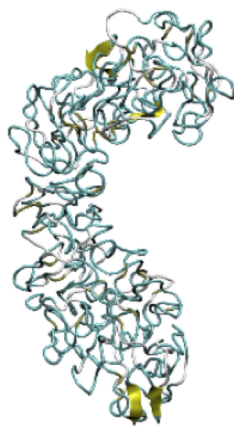**David L. Kaplan** (Tufts University)

General SITEP workflow

Progress: dynamic biomaterials

Full atomistic   Coarse-grained

Computational model → Experimental validation

Experimental predictions ← Structure, Dynamics, Function

7°C → 57°C

Differential scanning calorimetry

a) SE$_{8Y}$ Heat Flow, μW Temperature, K

b) S$_4$E$_{8Y}$ Heat Flow, μW Temperature, K

c) SE$_{8Y}$ 277 K 330 K 1.3 nm 4.3 nm Intensity, % Particle Size, nm

d) S$_4$E$_{8Y}$ 277 K 330 K 3.7 nm Intensity, % Particle Size, nm

Experimental Transition Temperature of 21°C (294 K)

Radius of Gyration, Å — Temperature, K
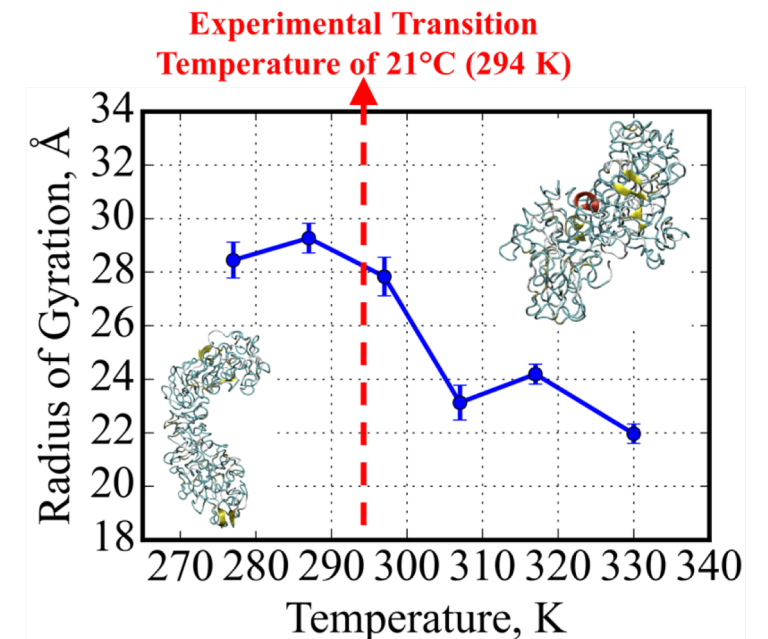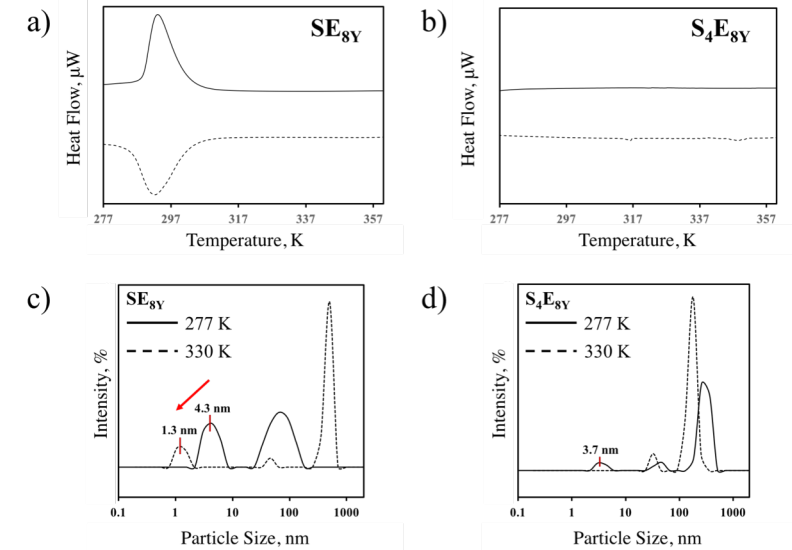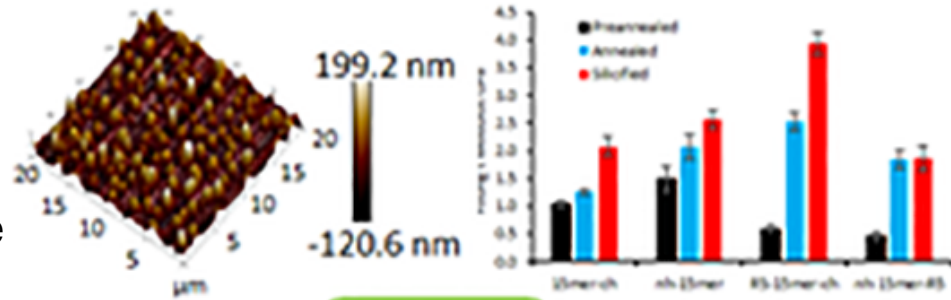
Progress: bio-mineral interface

Atomic Force Microscopy, mineralized film surface image

Silk film secondary structure analysis

Computational model
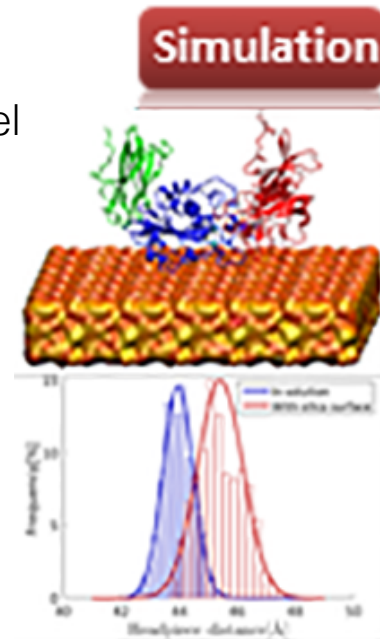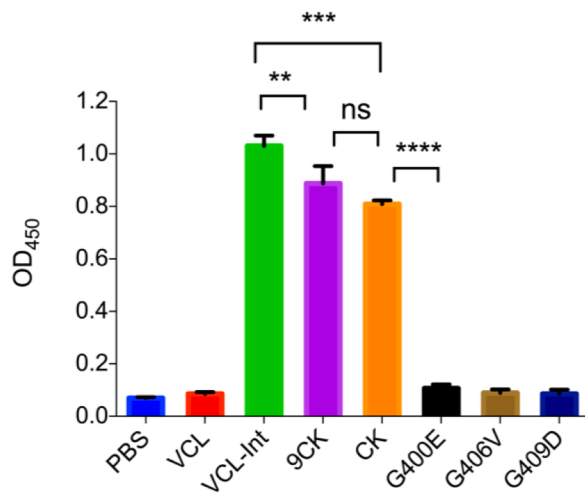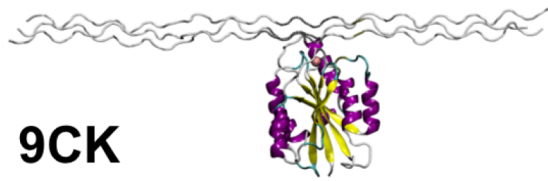
Gene and protein expression analysis

Progress: structural analysis of collagen

Full atomistic model

9CK

Loss of function

Computational model → Experimental validation

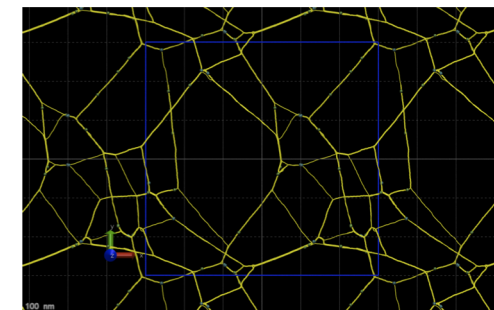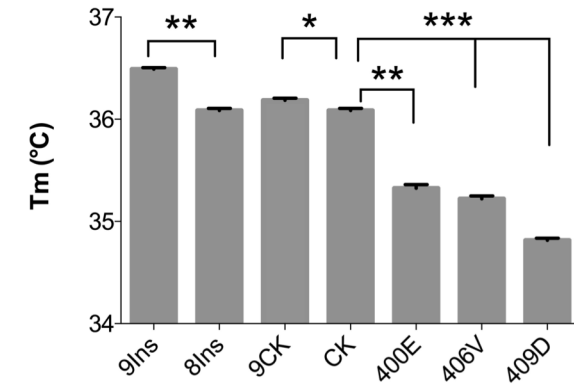Experimental predictions ← Structure, Dynamics, Function
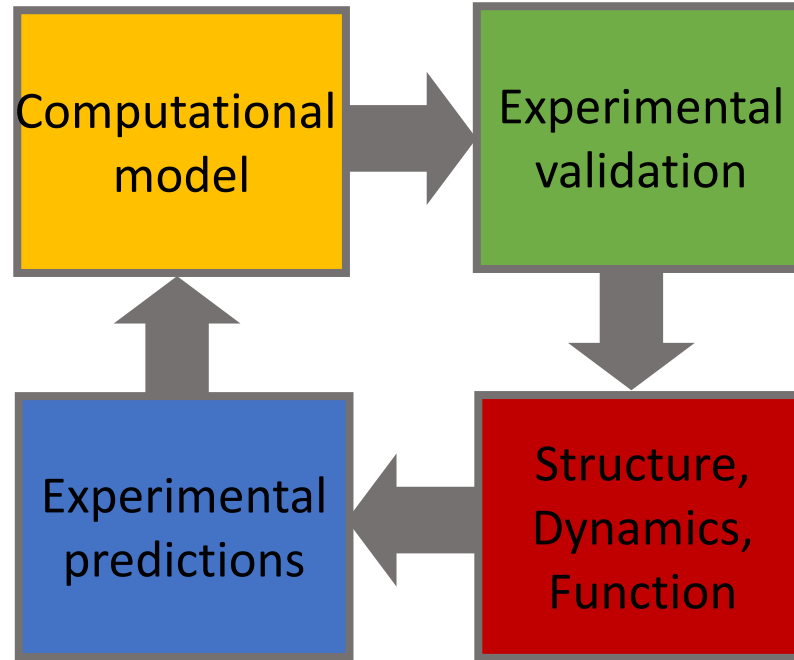
Thermal stability

Collagen membranes mechanical behavior

Shared to reproduce and reuse:

Videos:

- https://pubs.acs.org/doi/suppl/10.1021/acsbiomaterials.7b00292/suppl_file/ab7b00292_si_003.avi
- https://www.youtube.com/watch?v=qbm1RPn7Tdc&t=19s

Methods/papers:

- J Yeo, GS Jung, A Tarakanova, FJ Martín-Martínez, Z Qin, Y Cheng, Y-W Zhang, M J Buehler, Extreme Mechanics Letters 20, 112-124 2018
- J Yeo, GS Jung, FJ Martín-Martínez, S Ling, GX Gu, Z Qin, MJ Buehler, Physica Scripta 93 (5), 053003, 2018
- NG Rim, EG Roberts, D Ebrahimi, N Dinjaski, MM Jacobsen, Z Martín-Moldes, M J Buehler, D L Kaplan, J Y Wong, ACS biomaterials science & engineering 3 (8), 1542-1556, 2017

Experimental collaborations: shared models.

- Tony Weiss, University of Sydney, Australia
- Flavia Libonati, University of Milano, Italy
- Leila Deravi, Northeastern University, USA
- Guy Genin, Washington University in St Louis, USA

Web sites:

- http://lamm.mit.edu/silk-integrative-theory-experiment-project-sitep
- https://www.imagwiki.nibib.nih.gov/content/integrated-multiscale-biomaterials-experiment-and-modeling-group-imubeam

Additional initiatives going forward:

Tutorials to be posted on the web site:
- Crystallographic planes and use in modeling – e.g., per HA and silica work)

Checking with other colleagues outside the project
- Share models, and scripts

Further outreach on model credibility and reusability:
- MRS symposium, with a specific session on model credibility and reusability