Models to Predict Protein Biomaterial Performance

The model – Hierarchical models cover different material length scales to address biomateriomics – the nexus of advanced computation and simulation, theory and experiment to realize multiscale analysis of biological and biologically inspired materials and structures. We formulate *in silico* models of basic (universal) building blocks of different protein-based biomaterials (e.g., silk, elastin, collagen), and o define fundamental interaction rules, as well as environmental and assembly constraints; covering key themes at the core of biomaterial functions (e.g., mechanical properties, degradation lifetime, mineralization, sequence-disease states…).

What is new inside? Modeling of materials at hierarchical length scales to correlate molecular, meso- and macro-scale mechanics to protein-polymer features related to structure-function. Use of AI to drive materials discovery at multiple length-scales

How will this change current practice?

Biomaterial designs in silico, based on property targets and performance, to guide synthesis and functions. Improves polymer quality, reduces time from discovery to useful outcome, improves efficiency, saves resources, provides new fundamental rules governing design.

End Users – Scientists and engineers all stages of the materials implementation process – from sequence design to biological-regulatory approval processes.