Multiscale science of biological protein materials in extreme conditions and disease

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Biology exquisitely creates hierarchical structures, where initiated at nano scales, are exhibited in macro or physiological multifunctional materials to provide structural support, force generation, catalytic properties or energy conversion [1-3]. This is exemplified in a wide range of biological materials such as hair, skin, bone, spider silk or cells, which play important roles in providing key functions to biological systems [4-7]. This talk focuses on multiscale studies of deformation and failure of biological protein materials, used here to elucidate fundamental design concepts in order to understand physiological functions, disease mechanisms as well as to translate new material paradigms towards engineered nanomaterials.

Based on a multi-scale simulation approach, validated through multi-scale experiments, we explicitly consider the architecture of protein molecules across multiple scales, including the details of chemical bonding and explain how complex multifunctional properties of protein materials emerge. I will present a survey of recent studies of major classes of protein materials, including cellular protein networks, beta-sheet structures as found in spider silk and Alzheimer’s disease, as well as collagenous tissues that form the structure of tendon and bone. Case studies will be presented that illustrate size effects in protein materials, flaw-tolerance mechanisms, and applications of materials science to genetic diseases, showing how structural defects at the molecular level can have profound effects at the material behavior at larger scales. Analogies with engineered materials such as polymers, ceramics and metals in different geometries will be discussed, and new approaches towards the design of adaptable, mutable and active nanomaterials will be presented.
Figure 1: Experimental, theoretical, and computational tools for the characterization and modeling of deformation and failure of materials, plotted over their respective time and length scale domain of applicability. Adapted from [2].

References