Molecular Modeling and Design of Super-elastic and Self-healing Soft Materials

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Self-healing hyper-elastic soft materials can be accurately modeled, understood and designed using Molecular Dynamics (MD) simulations together with emerging techniques in data-science and machine learning. We have developed models of soft-matter systems using computationally efficient coarse-grained models that bridge atomic-to-mesoscopic length and timescales. I will describe two classes of soft materials that I have studied with these modeling techniques.

The first material system is superlattices that self-assemble from nanoparticles stabilized by selected soft organic ligands. These materials exhibit unique combination of functional properties relevant for applications in mechanical, optical, chemical detection, sensing and actuation. For example, PbS nanoparticles stabilized by oleic acid ligands were found to self-assemble into face-centered cubic crystals that demonstrate a remarkable degree of flexibility, with an elastic modulus of 2-3 GPa and the ability to retain crystalline order up to pressures of 40 GPa. These dramatic size changes enable broad tunability of the electronic/optical properties of the crystal by using pressure to tune the spacing between nanoparticle cores. Similarly, we found that thin membranes of Au-oleic acid superlattice stretch up to 90% strain without breaking and even completely self-heal when repetitively strained beyond the breaking point. *The second material system* is ordered structures of collagen self-assembled *in vitro.* The fundamental principles uncovered in this study are relevant for understanding the self-organization of numerous other biological macromolecules.

Badri Narayanan, Assistant Professor Mechanical Engineering, University of Louisville, holds the Ph.D. in Materials Science, Colorado School of Mines (2013). He previously was a Materials Scientist (2016-18) and Postdoctoral Associate (2014-16) at Argonne National Laboratory. His research centers on predictive, multi-scale modeling of functional materials and interfaces with applications to energy storage, catalysis and nano-electronics. His studies include extensive application of data-science and machine learning to accelerate discovery and design of materials. He is currently funded by the U.S. Department of Energy on studies of quantum materials, electrochemical interfaces and solid-state batteries. In 2017 he was awarded the Early Career High Impact Science Achievement Award from the National Energy Research Scientific Computing Center, and in 2020 he was awarded the Ralph. E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities.

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