Computational Material Design and Mechanical Behavior of Materials at the Molecular Level

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With the advent of the current millennium, the demands for novel structural materials with tailorable mechanical properties have been increasing every day. To incorporate revolutionary microstructural features in a material, it is essential to design a material from its building block level, i.e. from the molecular level. Moreover, strength and fracture properties of a material are also guided by the material's atomistic level bond-breaking and crack-formation mechanisms. Recently, high performance computational resources have become more accessible and greatly shifted the paradigm of materials research. In this seminar, I will discuss my recent studies on the computational material design and mechanical properties of soft and hard structural materials at the nanoscale. In particular, I will demonstrate 1) mechanical behavior of cytoskeleton, biological materials 2) materials for neuromorphic computing. Later, I will present my research to involve undergraduate students. Finally, I will provide a highlight of my future research directions and vision.