**Hierarchical nanomechanics of protein materials: Robustness and adaptability**

**by Prof. Markus Buehler**

**Date:** 26th June 2007 (Tuesday)  
**Time:** 11:00 am to 12:00 pm  
**Venue:** EA-06-05 (Seminar room)

**Abstract**

Proteins constitute critical building blocks of life, forming biological materials such as hair, bone, skin, spider silk or cells, which play an important role in providing mechanical stability for biological systems. However, the fundamental deformation and fracture mechanisms of biological protein materials remain largely unknown, partly due to a lack of understanding of how individual protein building blocks respond to mechanical load. All deformation and fracture processes begin with erratic motion of individual atoms around flaws or defects that may quickly evolve into formation of macroscopic fractures as chemical bonds rupture rapidly, eventually compromising the integrity of the entire structure. Here we use large-scale molecular dynamics (MD) simulations combined with statistical theories to develop predictive models of the deformation and fracture behavior of protein materials, exemplified in alpha-helical (AH) and beta-sheet (BS) protein structures. We review studies of spider silk – a natural fiber that can reach the strength of a steel cable, as well as intermediate filaments – an important class of structural proteins responsible for the mechanical integrity of eukaryotic cells, which, if flawed, can cause serious diseases such as the rapid aging disease progeria. Based on Bell’s theory, we derive a theoretical model that explicitly considers the hierarchical architecture of these proteins and chemical bonding, accurately predicting their unfolding behavior, providing a rigorous structure-property relationship. We analyze the fundamental deformation mechanisms of beta-sheets and the unfolding of alpha-helices due to mechanical cues. These two motifs represent the most abundant protein building blocks in biology, and thus, the development of a structure-property relationship is important for the understanding of many biological processes. We also report an analysis of the role of molecular defects at the on the overall protein behavior, illustrating concepts of silencing and activation of particular structural features at distinct hierarchical scales. We show that molecular defects are found universally and at a highly conserved location in intermediate filament dimers, and could play a critical role in enhancing the robustness of the filament networks against mechanical deformation. Further, our results provide strong evidence that the particular geometry of alpha-helical proteins can be explained based on Pareto’s principle, that is, that their structure leads to a maximized robustness at minimal use of building materials. While Pareto’s principle has been observed to apply to a wide range of natural and socio-economic phenomena, it has never been discussed in the context of protein materials. Our results reveal that this concept can also be used to explain the structure of proteins. Our studies elucidate intriguing material concepts that enable to balance strength, energy dissipation and robustness by selecting nanopatterned, hierarchical features.

**Professor Markus Buehler**

After obtaining his undergraduate education at the University of Stuttgart, Germany in Chemical and Process Engineering, Prof. Markus Buehler received his M.S. degree in Engineering Mechanics from Michigan Technological University, USA, in 2001. From 2001 to 2004 he worked at the Max Planck Institute for Metals Research in Stuttgart, Germany as a research assistant from where he also received his Ph.D. in Chemistry. From 2004 to 2005, Prof. Buehler held an appointment as the Director of Multiscale Modeling and Software Integration at the Materials and Process Simulation Center at the California Institute of Technology, overseeing multiscale method development and applications in modeling of small-scale materials phenomena. In 2005, he joined Massachusetts Institute of Technology (MIT) to assume a faculty appointment in the Department of Civil and Environmental Engineering. Prof. Buehler founded MIT’s Laboratory for Atomistic and Molecular Mechanics, where his research is focused on multi-scale modeling of complex hierarchical protein materials. He is currently the associate editor of the Journal of Computational and Theoretical Nanoscience and guest editor of the Journal of Materials Science. He has made significant contributions in the field of atomistic and molecular modeling of deformation and fracture of brittle, ductile and biological materials. His research has been highlighted in several journals, including the MIT Technology Review, New Scientist and Materials Today Prof. Buehler has received several awards, including the Materials Research Society Gold Graduate Student award and the National Science Foundation CAREER award. He has recently been invited to join the Frontiers of Engineering Symposium of the U.S. National Academy of Engineering.

**Dr Xue Jun Min**

ALL ARE WELCOME!