

From Computational Mechanics to Structural Biology and Its Engineering Applications

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In the era of bioengineering, not only state-of-the-art experimental technology, but also theoretical and computational approaches receive great attention as a means of optimal design and performance prediction of advanced bio applications. This talk will review how to bring the conventional framework of macroscale mechanics down to the level of nanoscale structural vibration and dynamics. In particular, a variety of coarse-graining modeling techniques known as elastic network model will be introduced with several examples from protein dynamics to DNA nanostructure design. Furthermore, it will be also discussed how to interpret harmonic vibration features of protein structures as well as their conformational changes in terms of biological functions. Lastly, ongoing research activities including DNA foldback intercoil structure as a promising pathway of homologous recombination and artificial water channel membrane for advanced biomimetic filtration technology will be addressed as good examples of simulation based bioscience and bioengineering, respectively.