Abstract:

The extraordinary biodiversity and complexity that evolution has produced from unicellular organisms to higher animals and humans within about one to two billion years is awesome. We are fascinated by the familiar and very complex and highly specialized organs - such as the eye, muscles, brain - all 'apparatuses' that perform their functions remarkably well. Nevertheless, evolution had already done its 'main work' on the unicellular organism: Without at least as highly specialized 'nano machines' - the proteins - not even microorganisms would be able to survive.

Almost all functions, e.g. photosynthesis for energy production in plants, various forms of movement, signal transmission and information processing, e.g. in the brain, sensor technology and recognition (smelling, tasting, seeing...), are performed by proteins whose perfection was already very advanced two billion years ago and often far exceeds that of our organs, not to mention our current technology. Atomistic computer simulations of the motion and dynamics of the atoms that make up the proteins, combined with sophisticated experiments, enable a better understanding of the underlying functional mechanisms.

We are beginning to realize that, already long ago, evolution 'invented' molecular electric motors, chemical factories, photocells, transformers, accumulators, 'Castor' transporters, and sensors.

The lecture gives an overview of the state of the art of atomistic computer simulations, and what we can learn about how proteins are 'manufactured' by ribosomes, how antibiotics interfere with bacterial ribosomes, and how molecular recognition and specific ligand binding works. We will, finally, take a more global view on the 'universe' of protein dynamics motion patterns and demonstrate that a systematic coverage of this 'Dynasome' allows one to better predict protein function.