Molecular Control Engineering: From Enzyme Design to Quantum Control

Whereas in the 20th century, chemists and physicists directed their attention toward the observation of atoms and molecular dynamics, in the early 21st century, they are teaming with engineers to manipulate these processes by directly controlling molecular dynamics in order to emulate and improve upon nature’s designs. This challenging goal requires application of the principles of engineering control and optimization to the structure and dynamical laws governing atomic and molecular motion. This talk will survey my group’s work in molecular-scale control and optimization, with an emphasis on two major topics: a) optimization of protein function. b) quantum control.

Natural evolution has succeeded at controlling chemical reactivity through the optimal design of catalytic proteins, or enzymes. We have shown that through computational design it is possible to produce, in a matter of minutes, the enzyme sequences that nature has selected over billions of years of evolution. Our current efforts to combat age-related diseases by redesigning sirtuin enzymes, the gatekeepers of human longevity, will be discussed. Our patented and licensed work on optimization of enzymatic reaction networks, which has led to the first FDA approved test of its kind for mental retardation in children, will also be described.

Quantum control is the only inverse problem in the control of chemical reactivity that has been rigorously solved. It involves the manipulation of delicate quantum wave interferences to optimally direct atomic and molecular dynamical phenomena for ultra-selective chemistry. By reducing the production of reaction by-products to the theoretical minimum, it may hold the ultimate answer to chemical sustainability (biological photosynthetic solar energy conversion, which achieves nearly 100% conversion efficiency, is based on quantum control). Our work on the foundations of quantum control theory and experiments, using state-of-the-art laser control systems, will be presented.