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SEMINAIRE DU GAP BIOPHOTONICS

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"Why is chemical synthesis and property optimization easier than expected?"

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Résumé:

The goals of chemical synthesis and property optimization may at first appear to be distinct from the control of molecular scale dynamical events with laser pulses. However, these subjects are intimately connected at a fundamental level through their common utilization of optimal control principles including at the quantum mechanical level. The presentation will first highlight the key concepts of laser driven quantum control achieving optimal performance, which is proving to be easier than expected. The talk will then transition over to considering the parallel goal of identifying optimal conditions for chemical and material synthesis as well as optimizing the properties of the products, which are often much easier to achieve than simple reasoning would predict. The potential search space is infinite in principle and enormous in practice, yet optimal molecules, materials, and synthesis conditions for many objectives can often be found by performing a reasonable number of distinct experiments. Considering the goal of chemical synthesis or property identification as optimal control problems provides insight into this good fortune. Both of these goals may be described by a fitness function J that depends on a suitable set of variables (e.g., reactant concentrations, components of a material, processing conditions, etc.). The relationship between J and the variables specifies the fitness landscape for the target objective. Upon making simple physical assumptions, the fitness landscape for chemical optimization can be shown to contain no local sub-optimal maxima that may hinder attainment of the absolute best value of J . This feature provides a basis to explain the many reported efficient optimizations of synthesis conditions and molecular or material properties. We refer to this development as OptiChem theory. The predicted characteristics of chemical fitness landscapes are assessed through a broad examination of the recent literature, which shows ample evidence of trap-free landscapes for many objectives. The implications of OptiChem theory for chemistry will be discussed along with the broader perspective encompassing the use of tailored laser fields for manipulating molecular phenomena.

