Dynamics and Structure of Molecular Fluids: A Symposium in Honor of Branka Ladanyi

When the general public thinks of chemistry, they envision reactions occurring in beakers and flasks filled with liquid solutions. Chemistry often focuses on the solutes in these chemical systems—but what enabled by photon absorption. Whether photoisomerization of a chroomophore or electron-electron transfer, all cases are studied (both theoretical and experimental) exploring the liquids, liquids in confined environments, microemulsions, supercritical fluids and molecular clusters. This symposium will highlight studies that aim to unravel the complex dynamics in these systems and phenomena at a microscopic level. The symposium has challenged scientists for generations and one that is critical for the comprehension of real chemical processes. These systems formed the basis of the far-reaching and significant contributions from the late Prof. Branka Ladanyi, whose scientific contributions added profoundly to the theory and modeling of complex environments such as interfaces, collaborations between theorists and experimentalists. This symposium will feature invited and contributed talks in honor and memory of Branka Ladanyi.

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Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

The National Nanotechnology Initiative began in 2001 in the U.S., catalyzing an enormous burst of research activity in the area of nanomaterials. The promise of the investment was predicated on new materials and applications that could not only stimulate science but also stimulate innovation, technology, and societal good in the form of the economy. A good question to ask in 2017 is: How far have we come? How well do we understand the fundamentals of nanomaterials, and how much of our knowledge has led to new technologies? Because the field of nanomaterials is so broad, this symposium will focus on plasmonic nanomaterials. The particular topics include metamaterials and information technology; surface chemistry, sensors, and diagnostics; plasmonic solutions to the energy problem; and plasmonic solutions for medicine. We aim to have at least one industrial speaker/entrepreneurial professor per session who can speak to the societal impact of the science and technology.

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Multicenter Molecules and Coupled Molecular Assemblies: Synthesis, Characterization, and Theory

The theme of this symposium is the design and characterization of systems of interacting multicenter molecules (i.e. molecules that support multiple electronic configurations). A classical example of a multicenter molecule is a mixed valence compound that contains a pair of metal sites that can change their oxidation state through electron transfer. Coupled molecular systems represent a new paradigm for information transfer and processing at the ultimate limits of the length scale—the single molecule. The charge distribution of a multicenter molecule is strongly coupled to that of neighboring molecules. This property can be exploited to create controlled interactions between molecules, potentially forming large-scale assemblies. The symposium will focus on the electronic, structural, and chemical characterization, and on the novel properties that can arise from interactions between multicenter molecules. A primary objective of this symposium is to foster discussion of new paradigms for utilizing multicenter molecules and coupled molecular assemblies toward new technology.

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Quantum Dynamics in Large Scale Systems

The symposium will bring together experts and young researchers who develop new approaches to quantum dynamics and quantum chemistry in extended systems. A broad range of topics focusing on fundamental challenges, as well as methodological and practical aspects of large-scale calculations in quantum chemistry will be covered.

The symposium will foster merging the two presently distant worlds: the field of stationary quantum calculations in large-scale systems and the field of ab initio simulations of quantum dynamical processes. The symposium will aim to stimulate interdisciplinary and complementary research efforts reaching and significant contributions from the late Pr. Nancy E. Levinson, Colorado State University, nancy.levinson@colostate.edu
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Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices and Catalysis on Interstellar Grains

Significant new experimental techniques have been developed during the last decade to investigate the interaction of ionizing radiation and of neutral atomic and molecular species with surface analogs of solids in the Solar System and in the Interstellar Medium (ISM). Investigation of these chemical processes provide fundamental insight into the molecular evolution of the interstellar medium, planet forming regions, and the origins of life. The interstellar medium is a complex mixture of atomic and molecular neutrals, ions, and radicals, interacting with solids in the Solar System and in the Interstellar Medium. Investigation of these chemical processes provide fundamental insight into the molecular evolution of the interstellar medium, planet forming regions, and the origins of life.

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Sunlight-driven Processes: Exposing the Mechanisms Behind Novel Photocatalytic and Productive Photocatalytic Activities

The proposed symposium offers an uncommon wide view of recent developments in the molecular- and electron-level understanding of sunlight-driven processes from biological systems to materials design. Light-induced processes fundamentally rely on using coupled electronic and nuclear motions enabled by photon absorption. Whether photoisomerization of a chroomophore or electron-electron transfer, all cases are driven by the initial absorbed photon energy which is then transduced into electronic and vibrational dynamics. Thus, the design and synthesis of molecules or molecular complexes that efficiently exploit light to drive wanted functions, must necessarily rely on the intimate knowledge of the mechanisms that efficiently converts the absorbed energy into specific electrons or atomic motions. The main target of the symposium is to provide an opportunity to discuss interdisciplinary and complementary research efforts for exploring the mechanisms underlying the exploitation of sunlight going from biological to engineering materials. Effort will be made to the understanding of the electronic, atomic and molecular details of these processes “resolved” via complementary experimental and computational approaches. The hope is to highlight how, presently, the mechanistic understanding of biological light-driven functions are, or might be, exploited in the development of functional materials going from light energy harvesting and storing materials to photocatalytic materials.

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