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ATOMS IN MOTION: CREATING AND CHARACTERIZING DYNAMIC CRYSTALLINE MATERIALS

A lecture in honor of the late Professor Philip Coppens

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In over 430 peer-reviewed publications, the late Professor Philip Coppens (1930-2017) is credited with critically important contributions in charge density and time-resolved X-ray diffraction methods. In both theory and practice, his contributions impacted virtually every aspect of high resolution electron density measurements: helium temperature experiments, data reduction, multipole modelling, combined analysis of charge and spin densities, derived electrostatic properties, multipolar data bases, and applications to chemical bonding and material science.

Image of late Professor Philip Coppens in his office. Photo credit: Nancy J. Parisi

Much of Philip's later work involved the development and application of time-resolved X-ray diffraction methods to monitor light-induced transformations in small molecule systems. His notable achievements in the area of photocrystallography include the structural determination of metastable intermediates in sodium nitroprusside, photochemistry in supramolecular systems, the development of software for the analysis and refinement of monochromatic and Laue X-ray diffraction, and the picosecond structural dynamics of organometallic complexes.

In addition to a brief remembrance of Philip, the lecture will showcase the exciting science involving the design, synthesis, and characterization of dynamic crystalline materials. Organic luminescent solids are an attractive alternative to current light emitting materials nearly all of which contain Pt, Ir, Re, or rare earth metals. Recently it has been shown that crystals of bromine-containing organic molecules are capable of exhibiting phosphorescence lifetimes of milliseconds and longer. Because of their long lifetimes, the luminescent materials are ideal for study by the pump-probe in-house time-resolved X-ray diffraction developed collaboratively by the Benedict and Coppens groups. Upon photo-excitation, crystals of 1,4-dibromo-2,5-bis(octyloxy)benzene exhibit a decrease in the intermolecular Br···Br contacts in the lattice. Attempts to rationalize these changes using computational modeling will be discussed along with some new results from other compounds in this class of organic light emitting molecules.

Recent results in which crystalline materials are used to convert light into useful work will also be described. The Benedict group is developing photo-switchable diarylethene-based linkers capable of transforming typically passive materials such as metal-organic frameworks into materials with chemical and physical properties that may be controlled externally with light. Recent successes in the synthesis of photo-responsive materials as well as challenges associated with transferring the solution state photo-reactivity into the solid-state will be presented.