

**Keywords:** charge density; photo-crystallography; spin density; time-resolved crystallography

## Introduction

Jason B. Benedict,<sup>a</sup> Yu Sheng Chen<sup>b</sup> and Claude Lecomte<sup>c\*</sup>

<sup>a</sup>Department of Chemistry, SUNY, University at Buffalo, Buffalo, NY, USA, <sup>b</sup>ChemMatCARS/CARS, University of Chicago, c/o APS/ANL, Chicago, USA, and <sup>c</sup>CRM2, IJL, Université de Lorraine and CNRS, BP 239, Vandoeuvre-les-Nancy, 54506, France. \*Correspondence e-mail: [claudel.lecomte@univ-lorraine.fr](mailto:claudel.lecomte@univ-lorraine.fr)

This special issue is dedicated to a lifetime of outstanding scientific achievements by Professor Philip Coppens. Originally a tribute to his recent retirement, this collection of papers – approved by Philip – was submitted by former students, postdocs, close friends and collaborators of Philip. Many of these individuals participated in a symposium ‘Advancing structural science: pushing the limits of X-ray crystallography’ held at the University at Buffalo in October 2016 that honored Philip’s scientific achievements (see <https://www.buffalo.edu/ubnow/stories/2016/10/coppens-symposium.html>). With Philip’s unexpected passing in June 2017, this collection of manuscripts has now become a remembrance of his impactful scientific legacy.

Among the earliest of pioneers of the field of charge density, Philip demonstrated that accurate high-resolution X-ray diffraction was an unparalleled experimental method for mapping and modeling electron density in crystals. In both theory and practice, his contributions impacted every aspect of charge density: helium temperature experiments, data reduction, multipole modeling, combined analysis of charge and spin densities, derived electrostatic properties, multipolar data bases, and applications to chemical bonding and materials science.

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. Several of his most notable achievements in the area of photocystallography 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.

Philip’s extensive influence on the community was felt well beyond his scientific literature and is beautifully described in an excerpt from Philip’s eulogy penned by one of his three sons, Eldad Coppens: ‘He was like a massive star that hurls through the universe with unrestrainable momentum and irrepressible energy affecting the course of everything in its orbit.’

We hope you enjoy reading this collection of manuscripts dedicated to the remembrance of Professor Philip Coppens (1930–2017).

Philip’s full eulogy is archived on the IUCr website at <http://www.iucr.org/people/crystallographers/philip-coppens-1930-2017>.

