Plenary Lectures

PL-O1

Crystallography in the 21st century: the age of electron?

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Crystallography as a scientific discipline has a history reaching at least four hundred years in the past. However, only in the 19thcentury it became a systematically studied field. In these early times, crystals were studied mostly by visible light. This "age of light" ended abruptly with the discovery of the diffraction of X-rays by crystals, starting the "age of x-rays" and the dramatic development of structural crystallography.

Electron microscopy and electron diffraction have long been considered useful, but mainly supplementary crystallographic techniques. However, we have been witnessing a number of important developments in the field of electron crystallography over the last decade that have changed the situation. First, it is the wide-spread availability of aberration-corrected transmission electron microscopes now allows a routine observation of – mostly inorganic – crystals at atomic resolution, including atomic-level chemical analysis. This gives an unprecedented insight into the structural arrangements at the smallest possible scale. Second, the development of the Cryo-EM technique for the reconstruction of molecular structures by high-resolution single-particle imaging brought a qualitative leap forward in our ability to understand the structures of biologically relevant molecular systems.

Somewhat in the shadow of these two ground-breaking developments stands another important progress in electron crystallography, namely the ability to solve and refine crystal structures from electron diffraction data. While some ten years ago an ab-initio solution of a crystal structure purely from electron diffraction data was limited only to special cases and was considered a very difficult challenge, today it has become an almost routine procedure. Hundreds of crystal structures have been solved from electron diffraction data, and some of them refined to accuracy comparable to the accuracy of x-ray structure analysis. The examples cover all types of structures, from oxides and metal alloys through minerals, zeolites and other framework materials, to metal-organic frameworks, organometallic compounds or pharmaceutically relevant organic materials, and even macromolecular crystals. This technique opens up a whole new realm of application of single-crystal structure analysis, because electron diffraction techniques are able to analyze crystals down to the size of a few nanometers.

There is no doubt that in the coming years x-ray diffraction techniques will remain dominant in the crystallographic research. However, seeing the rapid growth of importance of electron-based techniques, one may indeed ask a question: After the 19thcentury being the age of light and the 20thcentury being the age ofx-rays, is the 21st century going to be the age of electrons?

Keywords: electron crystallography, electron microscopy, nanocrystals

PL-O2

A tale in two parts: how a search for antivirulence compounds led to the discovery of a shapeshifting copper resistance protein

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Protein disulfide bonds are covalent links formed between sulfurs of cysteine sidechains. There is now overwhelming evidence to show that these inter-residue bonds are critical for Gram negative bacterial virulence [1]. This presentation describes how the structures of the bacterial machinery components that introduce disulfide bonds into folding proteins [2] have been used in the search for inhibitors [3,4,5]; and outlines the serendipitous discovery of a shape-shifting foldase [6] that is potentially useful for plug-and-play bionanotechnology.

References:

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