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Structure determination by correlated scattering

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In general what are measured on X-ray scattering are the intensities of X-rays. What is more if the scattering units are all identical and identically oriented; a measurable intensity is found from the unit cell even with relatively weak X-rays. Ingenious methods have been devised in X-ray crystallography for deducing the phases of the scattered X-rays and consequently the amplitudes of scattering. A Fourier transform of the scattered amplitudes gives the electron density of the unit cell and this often allows the structure to be deduced. The advent of the new X-ray sources such as those from an X-ray free electron laser (XFEL) allows a paradigm shift for the measurement of molecular structure. The increase in intensity of 10 billion-fold allows the possibility of structure determination even if proteins do not form crystals by scattering of individual molecules. A translation of the molecule gives rise to exactly the same intensities, but as rotation in general changes the intensities totally. However, even in the case of rotation a quantity called the angular correlations, while dependent on the structure, do not depend on the state of rotation or translation and is thus, ideally placed to allow structure determination of molecules typically injected into an XFEL in the form of particles of constant structure but unknown orientation or position. What is more, the absence of translational periodicity as in a crystal, allows the determination of the phases of the scattered amplitudes by an iterative phasing algorithm. We will discuss the use of angular correlations to determine the structures of proteins and viruses, with an XFEL.

Biography

D K Saldin has completed his DPhil from the University of Oxford, UK. After some Post-doctoral work at Oxford, he took up a position of a Research Fellow at Imperial College, London from 1981-1988. In 1988, he joined the Physics department of the University of Wisconsin-Milwaukee, where he currently holds the title of a Distinguished Professor.

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