CQSE Special Seminar

Weekly Seminar
Dec. 30, 2014 (Tuesday)

TIME   Dec. 30, 10:30am
TITLE   Solution of the X-ray phase problem in protein crystallography
SPEAKER Prof. Wu-Pei Su
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PLACE   Rm716, CCMS & New Physics Building, NTU

Abstract

  The X-ray phase problem is a long-standing problem in protein crystallography. It concerns the determination of a high resolution protein structure from the diffraction pattern of the protein crystal. Mathematically it is equivalent to the reconstruction of a real periodic function given the magnitudes (without the phases) of the Fourier coefficients plus other indirect prior knowledge of the function, such as the existence of a region where the function vanishes. A protein crystal is vastly different from a typical crystal that physicists are interested in. There could be tens of thousands of atoms in a unit cell, and hundreds of thousands of Bragg peaks in the diffraction pattern. It is therefore a daunting task to retrieve the atomic positions from the diffraction intensity. We have demonstrated that the phase problem is solvable for certain protein crystals, specifically crystals in which protein occupies less than half of the crystal volume. It is likely that the phase problem is also solvable for the rest of the protein crystals.