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X-ray Crystallography: It's Not Just about Structure Anymore

Abstract:

Symmetry is at the foundation of an idealized natural world, and the crystalline state might seem to exemplify this extreme order: mathematical symmetry operations can be used to describe a large perfect crystal in terms of a very small, repeating object called the asymmetric unit. The atomic details of this repeating unit can be determined experimentally by studying the X-ray diffraction pattern of the crystal. This approach has been invaluable for gaining insights into covalently and non-covalently interacting atoms and molecules. Real crystals are not perfect, and biomolecular crystal structures are models that best reproduce a subspace of the diffraction pattern. In practice, better agreement is found when structural disorder is taken into account via occupancies and atomic temperature factors. Typical protocols assume that atomic motion is independent, i.e., any given atom is uncorrelated with itself. This approximation allows the "perfectness" of the crystal to be maintained whereby the average electron density of the unit cell is stamped along the nodes of the crystal lattice. In reality, the atomic motions are correlated and this motion breaks the crystal symmetry spilling intensity into regions of the diffraction space that would be empty otherwise. In this talk, the effects of correlated motion on X-ray diffraction will be explored in detail, using several elastic network models of biological molecules; the potential of gaining information about the behavior of biological molecules in their crystalline state will be discussed.

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4:00 pm

Biotechnology Center Auditorium
425 Henry Mall