Freie Universität Berlin

Physikalisches Kolloquium des Fachbereich Physik
Arnimallee 14, D-14195 Berlin
Freitag, 14. Dezember 2018, 15 h c.t., Hörsaal A (R. 1.3.14)

Development of computational tools to characterize structure and dynamics of biomolecular systems from single molecule experiments

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Biological molecules are responsible for all life activities in the cells, and dysfunction of these molecules can cause severe diseases. Information on the structures of these biological molecules and their dynamics is essential to understand the mechanism of their functions, which can have a huge impact in medicinal applications.
The structures and dynamics of large biological complexes can be determined using a variety of experimental techniques, each providing information at different resolution. X-ray crystallography has been providing a large amount of structural information at detailed atomic levels. With recent progress in experimental techniques, Cryo Electron Microscopy (cryo-EM) provides 3D structural models near atomic-resolution. In addition, raw data from cryo-EM may now comprise millions of two-dimensional (2D) images of single molecules, which may represent distinct conformations of the molecule. Therefore, dynamics information could also be extracted from the 2D data. X-ray free electron laser (XFEL) is another exciting new technology that could significantly extend our structural knowledge of biological systems. Strong laser light from XFEL enables the measurement of single molecular complexes. However, for biological systems, due to their low diffraction power, signal to noise ratio is extremely low and interpretation of the data remains challenging.
Given progresses in single particle experimental techniques such as Cryo-EM and XFEL, new computational methods are also now needed to process and interpret data (millions of 2D images). We will discuss the development of hybrid computational methods that combine molecular mechanics and image data processing algorithms to derive structural and dynamical information of biomolecules from cryo-EM and XFEL data.