



## 复旦大学物理系物质科学报告

### **Conformational dynamics and protein machine: recognition, reaction, and signal transduction**

### Physics Department Colloquium

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Proteins are dynamic molecules. In the cell, the conformational ensembles of all soluble proteins are in equilibrium (time in-dependent) around their native states. To form a well-functioning machine with ordered movements, a protein unit has to recognize other molecules, to catalyze a chemical reaction, or to pass signal to other molecules in a dynamic way. The single molecule time-dependent dynamics of a protein is also decided by its conformational energy landscape, which is difficult to measure. Using different simulation approaches, we can examine various aspects of protein conformational dynamics to understand related protein functions. For example: (1) combination of MD simulation and bioinformatics analysis may reveal multiple modes of p53

protein assembly and DNA recognitions, which control cancer formation; (2) protein contact network analysis of protein dynamic trajectories helps to decode both kinetic and thermodynamic properties in signal transduction. New methodologies are needed to understand and characterize the subtle protein signal transduction within protein complex and protein interaction network in immune response.

**Time: 2:00pm, Tuesday, 2016.03.29**

**Location: Physics Building, Room 221B**

**(Cookies and coffee are served from 1:30 pm)**