

# Theoretical Understanding and Design of Molecular Functions of Proteins



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**Date & Time: 2017/12/15 (Fri.) 16:00-**

**Place: IMS Research Building Room 201**

This colloquium will also be held as a session of SOKENDAI Asian Winter School.

Protein functional processes involve dynamic molecular conformational changes of complex protein systems which often correlate with enzymatic chemical reactions. Hence molecular mechanism of enzymatic activities and coupling of the chemical reactions with protein molecular dynamics and flexibility underlying functional processes need to be revealed for understanding of molecular nature of protein functions. Furthermore, taking the protein flexibility into account is also crucial to designing novel functionalities of proteins through mutagenesis as mutations introduced often induce extensive conformational changes of proteins. In the talk, our recent molecular simulation studies on enzymatic reactions of protein complexes, activation processes of photoreceptor proteins, and analysis and design of color variants of photoreceptor proteins will be presented, and role of protein conformational changes and flexibility in protein functional processes will be discussed.

