



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
COLLOQUIUM

Growth of Amyloid Fibrils

by

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Date: February 17, 2012 (Friday)

Time: 4:00 - 5:00 p.m.

Place: L2 Science Centre, CUHK

(Light refreshments will be served 20 minutes prior to the colloquium.)

ALL INTERESTED ARE WELCOME

Abstract

Proteins form structured aggregates known as amyloid fibrils. The growth mechanisms of amyloid fibrils, which are implicated in a number of neurodegenerative diseases, are poorly understood. We have performed extensive all-atom molecular dynamics simulations to study the structural changes that occur in a random coil protein fragment from the yeast prion Sup35 and A β -peptide upon interaction with a preformed fibril. We show that the random coil to β -strand transition in the protein fragment as it becomes a part of the fibril occurs abruptly over a very narrow time interval. Amyloid fibrils further adopt a cross- β -spine structure in which the two β -sheets fully interdigitate to create a dry interface. Formation of such a dry interface is usually associated with self-assembly of extended hydrophobic surfaces. We studied the role of water and mechanistic differences in the dry interface formation between β -sheets formed from vastly different peptide sequences, one a polar sequence from the yeast prion Sup35 and the other a predominantly hydrophobic sequence from the A β -peptide.

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