

Atomic Modeling of the Putative Immature Retroviral Lattice using Molecular Dynamics

By

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Venue: Hilbert Space
Host: Assoc. Prof Chew Lock Yue

Abstract

After infecting a cell, a retrovirus like human immunodeficiency virus (HIV) will replicate its viral genome and produce thousands of identical Gag polyproteins. These polyproteins will subsequently oligomerize themselves into a hexameric lattice commonly referred as the immature Gag lattice. Once budded from the cell surface, the immature virus will undergo maturation by proteolytic cleavage of Gag. Obtaining an atomic structure of the immature Gag lattice has been elusive for many years. Recent advances in cryo-electron microscopy have yielded high resolution density maps and therefore enabled accurate computational modelings and simulations.

In this seminar, we present the first atomic model of an immature Gag lattice, using Rous sarcoma virus as the model system. This model was obtained using microsecond-long molecular dynamics simulations and tested by in vitro mutagenesis experiments. In light of our results, we discuss the recently published electron micrograph of the immature capsid of HIV.

Short Biography

Goh Boon Chong received his BSc in physics and math from Nanyang Technological University, under the supervision of Prof Chew Lock Yue. He is currently a PhD candidate at the University of Illinois at Urbana-Champaign in the group of Prof Klaus Schulten.