



THE CHINESE UNIVERSITY OF HONG KONG
Department of Physics
SEMINAR

What Can CHARMM-GUI Do for You?

by

Professor Wonpil IM
Presidential Endowed Chair and Professor of Biological Sciences
Lehigh University, USA

Date: October 22, 2025 (Wednesday)

Time: 10:30 – 11:30 a.m.

Place: Rm G25, Science Centre North Block, CUHK

ALL INTERESTED ARE WELCOME

Abstract

Since its original development in 2006, CHARMM-GUI (<https://www.charmm-gui.org>) has proven to be an ideal web-based platform to interactively build complex molecular systems and prepare their simulation inputs with well-established and reproducible simulation protocols for state-of-the-art molecular simulations using widely used simulation packages with various force fields. The CHARMM-GUI development project has been widely adopted for various purposes and now contains a number of different modules designed to set up a broad range of molecular simulation systems. Our philosophy in CHARMM-GUI development is less about providing the nuts and bolts of molecular modeling, but instead focused on helping users to achieve a task, such as building a membrane system or solvating a protein, by providing a streamlined interface. This design principle helps us to think of the workflow critically when designing the interface and new modules, which leads CHARMM-GUI to be accessible to users with little experience in modeling tools and remains useful to experts, especially for batch generation of systems. The CHARMM-GUI development project is still ongoing. CHARMM-GUI will continue to help expert and non-expert researchers from a broader range of the modeling and simulation community to build the complex molecular systems of their interest and prepare the input files for any general and advanced modeling and simulation through the large and unique scope of CHARMM-GUI functionality, allowing the research community to carry out innovative and novel molecular modeling and simulation research. In this talk, I will present the past, present, and future of the CHARMM-GUI development project, and some applications of specific modules will be also discussed.