

Computational Biology

Wonpil Im
Professor
10/22/2023

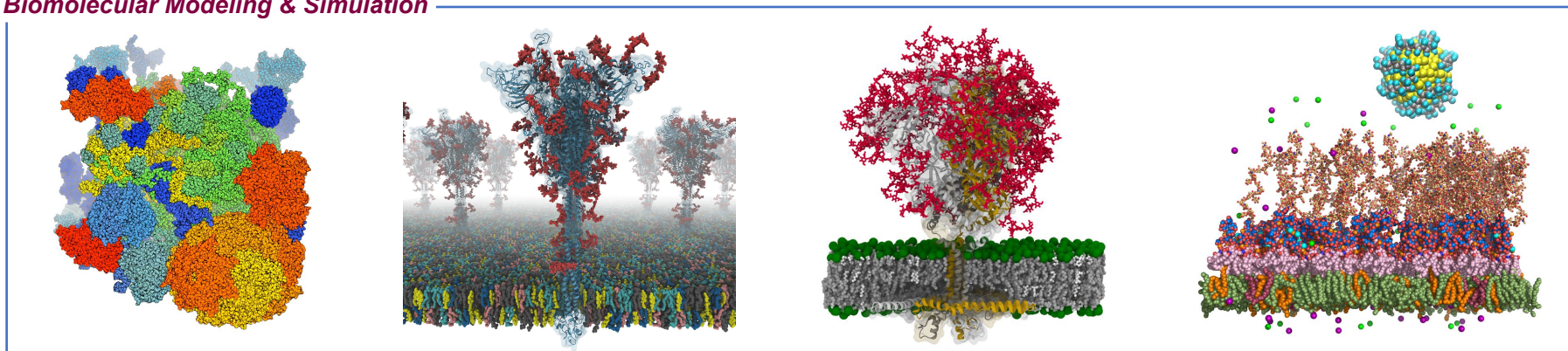


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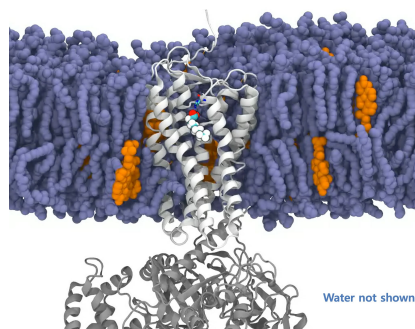
| **Department of Bioengineering**

Im Research Programs (<https://compbio.lehigh.edu>)

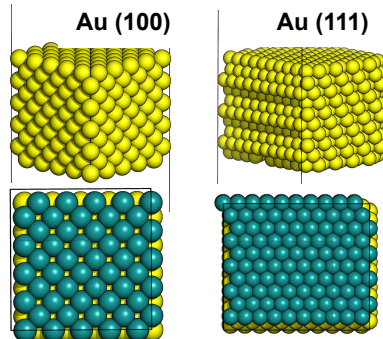
Biomolecular Modeling & Simulation



Computer-Aided Drug Discovery



Nanomaterial/Polymer Sciences



CHARMM-GUI Development

CHARMM-GUI
Effective Simulation Input Generator and More

CHARMM is a versatile program for atomic-level simulation of many-particle systems, particularly macromolecules of biological interest. — M. Karplus

about us | input generator | QM | archive | charmm docs | lectures | movie gallery | video demo | citations | updates | jobs & events | giving

Some licenses and job postings are now available. See [upload.log](#) for update history and [glzlog](#) for donation. [Contact](#) info is given below.

CHARMM-GUI Front Page

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CHARMM-GUI provides a web-based graphical user interface to generate various molecular simulation systems facilities and standardize the usage of common and advanced simulation techniques. Currently, CHARMM-GUI NAMD, GROMACS, AMBER, GENESIS, LAMMPS, Desmond, OpenMM, and CHARMM/OpenMM simulation are based on the CHARMM force fields.

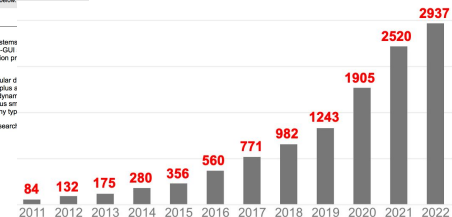
CHARMM-GUI is powered by CHARMM, an academic research program used world-wide for macromolecular dynamics (<http://www.charmm.org>). Its development began in the research group of Professor Martin Karplus and continues throughout the world with contributing developers. CHARMM performs standard molecular dynamics minimization with the potential energy functions for proteins, nucleic acids, lipids, carbohydrates, and various anions. CHARMM can be used for various chemical and conformational free energy calculations with many apps.

The CHARMM-GUI team hopes that the tools and materials offered here are useful and helpful for your research.

Academic users can obtain CHARMM freely from <http://www.charmm.org>.

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