

Studies of ion channel activation and modulation via computer simulation

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Ion channels are ubiquitous membrane-embedded transport proteins crucial for life. The central function of ion channels lies on their ability to selectively transport ions given the appropriate stimuli *e.g.* voltage, mechanical force, temperature or pH, and provided their regulatory gates are open. Gating mechanisms can be further modulated by ligands, a fact consistent with the fine tuning of their activity to molecular cues and organism demands. In this talk, by selected examples from our work, I will provide an overview of the current knowledge we have about activation, permeation and selectivity of ion channels and I will describe some of the technical challenges we face to model ion channels using atomistic computer simulation.

KEYWORDS: biophysics; membrane proteins; classical molecular dynamics; enhanced sampling techniques; free energy