سمینار هفتگي ماده چگال نرم

Computational Study of Structure and Function of Calcium Channels and Ion Barriers

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پژوهشگاه دانش‌های بنیادی

Ion channels are embedded proteins of the cell membrane. They open and close in response to different stimuli (gating mechanism) and some of them are permeable to specific types of ions (selectivity mechanism). When open, ion channels let the ion flux across the membrane, changing the ionic concentration on the two sides of the membrane. This concentration difference across the membrane leads to many essential physiological processes inside and outside the cell. Thus, there is a substantial interest to understand the ion channels' structure and function.

Nowadays, it has become possible to solve the crystal structure of many membrane proteins including ion channels. Once the crystal structures are known, it is possible to employ various computational techniques to get insights into the structure and function of ion channels, specifically at the atomic level.

In this thesis, we study two specific types of ion channels, using different computational techniques including MD simulations, BD simulations and free energy calculations.

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