سمینار هفتگی ماده چگال نرم

Polarization of Drug Molecules upon Membrane Translocation

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Abstract

Cancer is one of the most important health concerns that has no boundary, influences any organ and kills millions of people every year. Distinct characteristics of cancer cells such as adaptation to environmental selection forces and resistance to chemo-/radiotherapy are the major causes of frequent failures in cancer treatment. Despite of extensive research and progress in the field of drug design for cancer therapy, cancer is still a leading cause of death worldwide. To enhance the efficiency of anti-cancer drugs, it is most important to design the effective drugs. For effective modification, the cellular uptake of drug must be studied at atomic view. Since a detailed view of the interactions between drugs and membranes are often experimentally intractable, many different theoretical approaches have been used, including Quantum Calculations, Classical Molecular Dynamics (MD) and Monte Carlo. Although MD studies have previously been applied to the interactions between drugs and lipid bilayer membranes, important factors have been ignored. One of the ignored factors is the polarization state of the drugs. For that, we developed a new computational method to realistically study how drug molecules traverse cellular bilayers. Specifically, we developed a new methodology to account for electronic polarization, an important physical effect, unfortunately routinely ignored in large scale MD simulations due to the computational complexity. In this seminar, I will talk about our proposed method.

زمان: شنبه۹۹/۳/۲۴ ساعت ۱۵:۳۰

مکان(کلاس مجازی آقای دکتر اجتهادی):

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