سمینار هفتگی ماده چگال نرم

A molecular dynamics approach to study the thermal conductivity of amyloid beta in organic surface

Neda Rafieiolhosseini

Institute for Research in Fundamental Sciences (IPM), School of Nano Science

Abstract

The interaction of biomolecules with surfaces has been a topic of interest in many applications and hence, the target of many studies for decades. As a well-known organic surface, the cell membrane plays an important role in signaling, protecting, and the transportation of ions between the intracellular and the extracellular environments of a cell. In spite of the wide literature on the cell membrane, only a few has been dedicated to the thermal properties of the membrane. To find out how the interaction of membrane lipids with cholesterol and proteins affects the thermal conductivity of the membrane, we performed nonequilibrium molecular dynamics simulation of different model membranes. Moreover, we investigated the effect of asymmetric distribution of cholesterol in the two membrane leaflets on the membrane thermal conductivity. In the second part of this project, we investigated the interaction between amyloid beta peptide and the silica surface. Molecular dynamics simulations of a hydrophobic segment of the amyloid beta peptide near the amorphous silica water interface revealed that the peptide binds strongly to the surface with both hydrophobic and electrostatic interactions. These interactions affect the specific conformations and also the rotational mobility of the peptide. The orientation of the peptide relative to the surface is likely to play an important role in the fate of amyloid aggregation at the surface of silica nanoparticles. Results of this study apply to the development of new materials and advancement of selective treatment methods.

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