سمینار هفتگی ماده چگال نرم

Modelling and simulation of (Bio)molecules and nanostructured surfaces

Hesamodin Jami

Faculty of Engineering, School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, NSW 2006, Australia

Abstract

Molecular dynamics simulation (MD) is a vital tool to capture the dynamicity of biological molecules and atomistic insights. The prediction of the structural patterns generated during the self-organization of the layers of biomolecules on the surfaces relies on theoretical and computational knowledge behind them. As with any type of technology, however, these methods must be appropriately developed and applied if they are to provide realistic and valuable results. Such techniques are dependent on a description of how the molecules will interact – a force field – and are prevalent in materials chemistry, biochemistry and biophysics. The initial purpose of this study was to explore the mechanisms of biomolecules with surfaces using MD simulation and crosscheck with experimental results.

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مکان(کلاس مجازی آقای دکتر اجتهادی) :

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