

С Ъ О Б Щ Е Н И Е

На **20 октомври 2017 г. (петък)** от **11:00 часа** в зала „Болцман” на **ИФХ-БАН**, ще се проведе заседание на Колоквиума със следния дневен ред:

1. Доклад на Николай Панчев на тема:

„The role of canonical ensemble in predicting the toluene film structure under external electric field”

Formation of water-in-oil emulsions is common during the gasoline production. A thin oil film is formed to stabilize the emulsion when two drops approach each other. The demulsification requires rupturing of this thin liquid film usually by applying a strong electric field. Because the interest in rupturing mechanism is still vivid and needs a fundamental understanding, the present study has pursued the mechanism of film rupture by implementing the Molecular Dynamics method, which enables details at a molecular level. Two canonical ensembles, NVT and NPT were used to determine the strength of the field necessary to rupture the film. We observe a decreased film stability within the NPT ensemble in comparison to the NVT ensemble. As a result, the film is ruptured at a weaker electric field, i.e. 75 mV/nm instead of 120 mV/nm in the NVT ensemble. We show that the external field induces charge accumulation at the film interfaces, the charge increases with the field increase accompanied by a non-homogeneous film thinning. The film ruptures due to surface charge density gradient.

2. Разни (съобщения, организационни и др. въпроси).