Contribution ID: **927** Type: **Oral**

Raman spectroscopy, neutron scattering and MD simulation combined study of cholesterol and melatonin effects in lipid bilayer

Tuesday, 12 October 2021 10:45 (15 minutes)

We have studied the effect of cholesterol and/or melatonin on the static and dynamical properties of DPPC and POPC-based phospholipid bilayers utilizing neutron scattering techniques and Raman spectroscopy. We report that cholesterol induced an increase in bilayer thickness, while melatonin induced a decrease in bilayer thickness in the three-component systems of lipid/cholesterol/melatonin. Commensurately, by evaluating the projected area of lipid, we demonstrate its decrease with an increasing concentration of cholesterol, and its increase with an increasing concentration of melatonin. The demonstrated condensing effect of cholesterol and the fluidizing effect of melatonin appear in an additive manner upon their mutual presence.
Raman spectroscopy is known as a very sensitive instrument for probing conformational changes manifested in vibrational spectra of biological samples under certain conditions. The analysis of the obtained Raman spectra for DPPC was done in the certain part of the fingerprint region, specifically 1030-1150 cm-1, as it is known to be sensitive to trans/gauche conformations. We evaluated spectral weights (i.e., integrated areas) of three dominant Raman bands of DPPC (1062 cm-1, 1096 cm-1, 1127 cm-1) for estimating the order/disorder dynamics in our systems.
As expected, based on the two-component systems of lipid/cholesterol or lipid/melatonin studied previously, we show the impact of cholesterol and melatonin being opposite and competitive in the case of three-component systems of lipid/cholesterol/melatonin. It has been revealed that the effect of cholesterol appears to prevail over that of melatonin in the case of structural properties of DPPC-based bilayers, which can be explained by its interactions targeting primarily the saturated lipid chains. As a result of our studies and evaluations of the trans / gauche conformations ratios, it was shown that the dynamics of the studied three-component lipid-cholesterol-melatonin systems demonstrates a balanced competing effect of the two additives used in this study.

Primary author: ARYNBEK, Yersultan (JINR, INP, KazNU)

Co-authors: Mrs VOROBYEVA, Maria (JINR); Mr MAMATKULOV, Kakhramon (JINR); Mr ARZUMANYAN, Grigory (JINR); Mr KUCERKA, Norbert (JINR)

Presenter: ARYNBEK, Yersultan (JINR, INP, KazNU)

Session Classification: Condensed Matter Physics

Track Classification: Condensed Matter Physics