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## The dynamical properties of DPPC lipid bilayer: Raman spectroscopy characterization of the impact of cholesterol and melatonin

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### ABSTRACT

*We have studied the impact of cholesterol and/or melatonin on the dynamical properties of phospholipid bilayers made of dipalmitoylphosphatidylcholine (DPPC) by Raman spectroscopy and complemented the experimental results with MD simulation. Raman spectroscopy is known to be a sensitive instrument for probing conformational changes manifested in the Raman spectra of biological samples under certain conditions. It is well known that cholesterol has a condensing effect, namely it is capable of ordering the hydrocarbon chains of lipids, while melatonin is supposed to be a fluidizing one. The analysis of the obtained Raman spectra was done in the fingerprint region of 1030-1150  $\text{cm}^{-1}$  as it is known to be sensitive to trans/gauche conformations. The normalized Raman spectra in this region with the three dominant Raman bands for our system are shown in Figure 1a and 1b for three different concentrations of the components. We evaluated spectral weights (i.e., integrated areas) of three of these lines for estimating the order/disorder dynamics in our systems. In particular, we calculated the ratio of spectral weights at 1127  $\text{cm}^{-1}$  to that at 1096  $\text{cm}^{-1}$  ( $1127/1096$ ) for evaluating the ordering effect of cholesterol, while the ratio of spectral weights at 1062  $\text{cm}^{-1}$  to that at 1096  $\text{cm}^{-1}$  ( $1062/1096$ ) for evaluating the disordering effect of melatonin. As a result of our studies, it was revealed the effect of the cholesterol addition to the DPPC bilayers is modulated clearly by the additional presence of melatonin. This can be seen in the declining steepness of the trans/gauche ratio changes as a function of cholesterol concentration in the case of DPPC bilayers loaded with increasing amount of melatonin. Thus, the vibrational dynamics of lipid chains appears to be affected directly and similarly by both cholesterol and melatonin. The cholesterol clearly increases the order of lipid chains, and melatonin introduces disorder.*

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### Biography

Maria Vorobyeva is junior researcher of International Intergovernmental Organization Joint Institute for Nuclear Research. In the last three years, she has been very actively involved in lipid-protein interactions in model lipid membranes. Whereas the addition of various molecules to the membrane can change its physical properties and alter its structure, that in turn may affect its functionality. It is thus crucial to know the origin of these changes, and understand the intermolecular interactions responsible for embedding the various additives to the membrane. Of course, the influence of membrane functionality can go in both directions.