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Dynamics of beta-amyloid peptide in cholesterol superlattice domain ANTON SMIRNOV, QING ZHU, MARK VAUGHN, RAJESH KHARE, K. CHENG, Texas Tech University — Presence of beta-amyloid peptide (beta-A) plagues in membranes of neuron cells is a clinical signature of Alzheimer disease. The onset of beta-A peptide aggregation occurs via a conformational transition from an alpha-helix state to a beta-sheet state. A gradual build-up of beta-A content in the neuronal extracellular space is another characteristic of the beta-A plague formation. Hypothetically, both the pathological conformation and the predominant localization of the beta-A can be a result of specific dynamic characteristics of the interphase between cellular membrane and extracellular milieu. In this study, the beta-A interphase problem has been investigated using a virtual membrane model implemented on the base of GROMACS molecular dynamics simulation package. The detailed folding pattern of beta-A has been examined using a novice interphase model comprised of a cholesterol supperlattice membrane and two water layers.

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