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Computational Characterization of Electronic Charge Transfer in Interfacial Phospholipid-Water Layers

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Abstract : Existing signal transmission models, although undoubtedly useful, have proven insufficient to explain the full complexity of information transfer within the central nervous system. The development of transformative models will necessitate a more comprehensive understanding of neuronal lipid membrane electrophysiology. Pursuant to this goal, the role of highly organized interfacial phospholipid-water layers emerges as a promising case study. A series of phospholipids in neural-glial gap junction interfaces as well as cholesterol molecules have been computationally modelled using high-performance density functional theory (DFT) calculations. Subsequent 'charge decomposition analysis' calculations have revealed a net transfer of charge from phospholipid orbitals through the organized interfacial water layer before ultimately finding its way to cholesterol acceptor molecules. The specific pathway of charge transfer from phospholipid via water layers towards cholesterol has been mapped in detail. Cholesterol is an essential membrane component that is overrepresented in neuronal membranes as compared to other mammalian cells; given this relative abundance, its apparent role as an electronic acceptor may prove to be a relevant factor in further signal transmission studies of the central nervous system. The timescales over which this electronic charge transfer occurs have also been evaluated by utilizing a system design that systematically increases the number of water molecules separating lipids and cholesterol. Memory loss through hydrogen-bonded networks in water can occur at femtosecond timescales, whereas existing action potential-based models are limited to micro or nanosecond scales. As such, the development of future models that attempt to explain faster timescale signal transmission in the central nervous system may benefit from our work, which provides additional information regarding fast timescale energy transfer mechanisms occurring through interfacial water. The study possesses a dataset that includes six distinct phospholipids and a collection of cholesterol. Ten optimized geometric characteristics (features) were employed to conduct binary classification through an artificial neural network (ANN), differentiating cholesterol from the various phospholipids. This stems from our understanding that all lipids within the first group function as electronic charge donors, while cholesterol serves as an electronic charge acceptor.

Keywords : charge transfer, signal transmission, phospholipids, water layers, ANN
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