“Electromechanical Coupling in Lipid Membranes: Potential-induced curvature and neuronal heating from molecular simulations”

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Lipid membranes are liquid crystals, and an externally applied electrostatic potential should bend a membrane and vice versa. We measure the bending of a membrane upon external application of an electrostatic potential in a coarse-grained lipid model. We will also demonstrate the reverse effect using an all-atom model. When an action potential (a change in the transmembrane electric field) passes through a neuron, heat is first produced and then reabsorbed by the neuronal membrane, resulting in a small measurable temperature spike. I will describe the thermodynamics and molecular features of this phenomenon using a coarse-grained molecular dynamics approach. We find that the potential energy converted to heat is initially stored mainly in the imbalanced ion distribution across the membrane and the reversible elastic energy of the membrane has only a minor role to play. Time permitting, I will also talk a little bit about allosteric conformational control by a single cholesterol molecule in the conformational dynamics of the transmembrane Niemann-Picks Type C1 protein.