Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths

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Journal of Biomolecular Structure and Dynamics, April 2018, Taylor & Francis DOI: 10.1080/07391102.2018.1453376

Examining membrane damage due to traumatic brain injury-related deformations

What is it about?

Traumatic brain injury (TBI) is a widespread and extremely harmful form of injury. We have quantified the effect that complex deformation states due to TBI could have on a simple membrane through use of the molecular dynamics simulation method and provide the nanoscale basis for developing and implementing a multiscale physics-based material model for brain injury.

Why is it important?

Our findings show that the applied strain state has a significant effect on the membrane's mechanical and damage response and provides the basis for adding a physiological aspects to finite element material models. This finding is important because standard finite element material models only account for the mechanical deformation with no indication of cellular or tissue injury.

Perspectives

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The idea of using internal state variable models for metals and other materials to capture lower length scale phenomena is relatively mature. Applying this idea to biological systems allows the addition of injury-related physiological effect that can be tied to mechanical deformations. This perspective provides a unique way to examine injury that will better inform safety equipment design and guidelines via simulations.

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