



“Atomic-scale insights into membrane and membrane protein structure and function from molecular simulations“

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Abstract:

Membranes and membrane proteins are central to many key processes of life. Accurately modeling such systems at the molecular scale requires to overcome many challenges and to resort to a combination of diverse methods. I will discuss selected examples both from a methods point of view and in terms of biological and technological applications involving ion channel function and modulation by the membrane, membrane fusion related systems, hybrid to full coarse graining and incorporation of hydrodynamic effects.