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Surface Assessment via Grid Evaluation (SuAVE): A Tool to Analyze Curvature-Dependent Properties in Membranes

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Lipids self-assemble into diverse spatial arrangements according to chemical structure, lipid composition, and external variables (e.g. water content, temperature, pressure and salt). The transition between these phases requires sizeable changes in membrane curvature. In the last decades, computational simulation has emerged as a valuable method to complement experimental techniques to study membrane processes at the molecular scale. Considerable improvement in the quality of molecular models and continuous progress on the development of hardware and software has increased the predictability power and expanded the spatio-temporal scales accessible to computational simulations. However, the structural characterization of membrane phase transitions remains a challenging issue in many fronts. In this report, we are concerned about the accurate description of curvature-dependent properties for membranes undergoing phase transition from lamellar to non-lamellar (i.e. micellar, vesicular) arrangements. We have developed the program SuAVE (Surface Assessment Via grid Evaluation) for the precise and efficient calculation of several structural properties which are dependent of the surface curvature of the system such as the area and volume per molecule, membrane thickness, surface topology maps, density profiles, curvature order parameters and Gaussian curvatures. We demonstrate the accuracy of SuAVE numerical methodology through the analysis of the Lipid-A chemotypes assembled in distinct structural arrangements. We show that SuAVE provides a more accurate description of the structural properties of highly curved as well as closed surfaces compared to conventional tools for analysis of MD simulations.