Tilting Operator for Phospholipidic Molecular Domains at the Liquid-Gas Interface

Adel F. Antippa
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Abstract
We derive a coordinate independent operator expression for the Tilting Operator of molecular domains at the liquid-gas interface. The domains are made up of phospholipidic molecules modeled as spherocylinders. The molecules of the domain are oriented parallel to each other. The centers of symmetry of the molecules form a lattice. The Tilting Operator keeps track of the deformations suffered by this lattice as the domain molecules are tilted relative to the normal to the interface. The results obtained are important for dynamic calculations of inclination dependent collective film characteristics, as in the simulation of surface density versus surface pressure curves in a Langmuir film. The tilting operation can be decomposed into three separate simple operations: A global rotation, a local oblique realignment, and a global vertical translation.