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Adapting phase-switch Monte Carlo method for flexible organic molecules SALLY BRIDGWATER, DAVID QUIGLEY, Univ of Warwick — The role of cholesterol in lipid bilayers has been widely studied via molecular simulation, however, there has been relatively little work on crystalline cholesterol in biological environments. Recent work has linked the crystallisation of cholesterol in the body with heart attacks and strokes. Any attempt to model this process will require new models and advanced sampling methods to capture and quantify the subtle polymorphism of solid cholesterol, in which two crystalline phases are separated by a phase transition close to body temperature. To this end, we have adapted phase-switch Monte Carlo for use with flexible molecules, to calculate the free energy between crystal polymorphs to a high degree of accuracy. The method samples an order parameter $\mathcal{M}$, which divides a displacement space for the N molecules, into regions energetically favourable for each polymorph; which is traversed using biased Monte Carlo. Results for a simple model of butane will be presented, demonstrating that conformational flexibility can be correctly incorporated within a phase-switching scheme. Extension to a coarse grained model of cholesterol and the resulting free energies will be discussed.

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