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Interfacial adsorption and aggregation of amphiphilic proteins

DAVID CHEUNG, University of Warwick — The adsorption and aggregation on liquid interfaces of proteins is important in many biological contexts, such as the formation of aerial structures, immune response, and catalysis. Likewise the adsorption of proteins onto interfaces has applications in food technology, drug delivery, and in personal care products. As such there has been much interest in the study of a wide range of biomolecules at liquid interfaces. One class of proteins that has attracted particular attention are hydrophobins, small, fungal proteins with a distinct, amphiphilic surface structure. This makes these proteins highly surface active and they recently attracted much interest. In order to understand their potential applications a microscopic description of their interfacial and self-assembly is necessary and molecular simulation provides a powerful tool for providing this. In this presentation I will describe some recent work using coarse-grained molecular dynamics simulations to study the interfacial and aggregation behaviour of hydrophobins. Specifically this will present the calculation of their adsorption strength at oil-water and air-water interfaces, investigate the stability of hydrophobin aggregates in solution and their interaction with surfactants.

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