Hydrophobins at the water/air interface: A model system for protein self-assembly.

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Hydrophobins are a family of proteins that are characterized by a large exposed hydrophobic region, which makes them strongly amphiphillic. Hydrophobins of class II self-assemble into membranes at a water/air or water/oil interface where they form long ranged ordered hexagonal structures [1,2]. However the atomic details of the lateral assembly process at the interface remain widely unknown. Furthermore due to the reduced dimensionality and the high stability of the individual monomers, hydrophobins provide a simplified model system for studying assembly processes of proteins in general. In this project, we aim to understand the free-energy landscape and the kinetics of the formation of monolayers of HBFI at the water/air interface using atomistic and coarse-grained molecular dynamics simulations. In this early stage of the project, we focus on the formation of HFBI dimers and trimers by combining free MD simulations with Markov state models. The long-term goal is to simulate the entire assembly process in atomic detail.

[1] Linder, Markus B. "Hydrophobins: proteins that self assemble at interfaces." Current Opinion in Colloid & Interface Science 5.14 (2009): 356-363.

[2] Hähl, Hendrik, et al. "Pure protein bilayers and vesicles from native fungal hydrophobins". Advanced Materials 29.1 (2017): 1602888.