Molecular dynamic simulations of hydrophobins: pure-protein bilayers and lipid-protein interactions

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Hydrophobins are a family of proteins characterized by a large exposed hydrophobic region, rendering them highly amphiphilic. Class II hydrophobins such as HFBI self-assemble into monolayers at water-air or water-oil interfaces, revealing long-range ordered hexagonal 'honeycomb' structures[1]. This property allows for the preparation of pure-protein bilayers and vesicles [2] with unexpectedly low permeability for water and ions. To provide a molecular explanation for these properties, we carried out atomistic and coarse-grained molecular dynamics (MD) simulations of HFBI bilayers. Our results indicate that the proteins have to rearrange upon monolayer contact in order to form a stable dense bilayer.
In contact with lipid bilayers, hydrophobins were found to modulate the stability of the membrane in electroporation experiments. Coarse-grained simulations suggest that the proteins aggregate inside the pore and bind to the exposed hydrophobic membrane core, therefore leading to the observed stabilization.

[1] Lindner,M.B. Curr. Opinion in Colloid & Interface Science 14,356-363 (2009)

[2] Hähl et.al. Advanced Materials, 29, 1602888 (2017)