Theoretical Modeling of Dynamic Self-Assembly of class II Hydrophobins from T. reesei at the Air-Water Interface

Neda safaridehkohneh[1], *Hendrik Hähl*[2], *Jonas Heppe*[2], *Karin Jacobs*[2], *Ludger Santen*[1]

[1]*Department of Theoretical Physics, Saarland University, 66041 Saarbrücken, Germany, and* [2] *Department of Experimental Physics, Saarland University, 66041 Saarbrücken, Germany*

Hydrophobins are amphiphilic proteins which for instance assemble at the interface between aquas phase and hydrophobic phase, e.g. at the air-water interface. We investigate the dynamics of interfacial self-assembly of wild-type hydrophobins HFBI and HFBII both experimentally and theoretically. Experimentally, the kinetics were measured by monitoring the accumulated mass at the interface via non-destructive ellipsometry measurements. The measured kinetics for wild-type HFBI and HFBII showed not the expected typical Langmuir-type behavior but linear kinetics for a monolayer formation. In order to clarify the underlying microscopic mechanism, we introduce a stochastic model. The model includes electrostatics and van der waals interactions. Also the model includes microscopic movements in the air-water interface and in the solution. In our model, proteins are accumulated in the interface via two-step adsorption, i) pre-adsorption, in which proteins adsorb from the solution to the subsurface and ii) final adsorption from subsurface to the interface. We showed that the experimental kinetics can be reproduced if the pre-adsorption is sufficiently low enough compare to the diffusion.