

# $\beta$ -Lactoglobulin at the Water-Air Interface: MD Simulations on Different Time and Length Scales

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Second order spectroscopic techniques allow to selectively probe properties of molecules adsorbed to surfaces or interfaces, rather than bulk properties. E.g., sum frequency generation (SFG) has been used to study the proteins that stabilize foams formed by milk or whey. Additionally, ellipsometry provides information on the layer thickness of the adsorbed species. These experimental methods provide information on the order and layer thickness of the molecules adsorbed to the interface, over a range of pH values. [1] However, many of the molecular details of the aggregation and surface adsorption process remain unclear. Here, we use atomistic and coarse grained molecular dynamics simulations to investigate the aggregation and surface adsorption of beta-lactoglobulin in aqueous solutions at different pH values. We also investigate the influence of the electrolyte used.

[1] K. Engelhardt, A. Rumpel, J. Walter, J. Dombrowski, U. Kulozik, B. Braunschweig, W. Peukert, *Langmuir* **2012**, *28*, 7780–7787.