Ion and pH Effects on Foam Protein Aggregation

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Second order spectroscopic techniques allow to selectively probe properties of molecules adsorbed to surfaces or interfaces, rather than bulk properties. Sum frequency generation (SFG) is used to study the proteins that stabilize foams formed by milk or whey, thus providing information on the order of the molecules adsorbed to the interface. [1,2] Additionally, ellipsometry provides information on the layer thickness of the adsorbed species and the oligomerization state of a protein in the bulk can be examined by analytical ultracentrifugation. However, many of the molecular details of the aggregation and surface adsorption process remain unclear. Here, we use atomistic molecular dynamics simulations to investigate aggregates of beta-lactoglobulin in aqueous solutions at different pH values and in different electrolytes.

[1] K. Engelhardt, A. Rumpel, J. Walter, J. Dombrowski, U. Kulozik, B. Braunschweig, W. Peukert, *Langmuir* **2012**, *28,* 7780-7787.
[2] K. Engelhardt, M. Lexis, G. Gochev, C. Konnerth, R. Miller, N. Willenbacher, W. Peukert, B. Braunschweig, *Langmuir* **2013**, *29*, 11646-11655.