Fundamental Mechanisms on the Complexation of Milk Proteins

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Milk proteins have a rich diversity of physical chemistry and biodegradable properties which makes them appealing for different food and pharmaceutical applications. The interaction and complexation of these proteins is the clue to an efficient use as {\it e.g.} food additives. The protein-protein interaction is to a large extent governed by solution pH and salt concentration. Theoretical models and Monte Carlo simulations were employed here in order to gain novel insight into the fundamental mechanisms of milk protein complexation under different conditions. As such, these techniques are a valuable tool for the nascent soft matter approach of the food and pharmaceutical sciences offering a rational approach to describe, explain and control complexation mechanisms that affect the biological and practical functions. This is exemplified here by different examples. For instance, the interactions between alpha-lactalbumin, beta-lactoglobulin and lactoferrin were investigated. The comparison between free energies associated with the complexation of alpha-lactalbumin--lactoferrin and beta-lactoglobulin--lactoferrin at different pH and ionic strengths explains the experimental observation that the latter but not alpha-lactalbumin—lactoferrin forms a complex.
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