Nanoscale modelling of biomolecules in food science applications

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ABSTRACT: In the food industry, anhydrous triacylglycerol (TAG) molecules find extensive use as edible oils. This complex molecular environment contains polycrystalline particles composed of TAG molecules, and their networks, in anhydrous TAG oils. Recently, crystalline nanoparticles (CNPs) have been identified as the fundamental components of solid fats in oils. Modelling of such complex liquid environments present significant challenges. Our approach is to simplify the model to address a key issue in food science and technology: the "oil binding capacity" of a system of such edible oils. Oil binding capacity is an important concept regarding the ability of fat particles to retain oil, and the ability of these CNPs to bind oil is important in designing healthy foods. We have carried out atomic scale molecular dynamics computer simulations to understand the physics of oil binding capacity and elucidate the physical structures of liquid oil between a pair of solid surfaces. Specifically, we have modelled triolein oil in a confined nanoscale space between two tristearin surfaces. The intent is to attempt to shed light on whether, apart from the possible higher cost of creating single-component systems, those edible oils that find use in modern food technology must contain a mix of solid fats and complex many-component fluids in order to possess a high oil binding capacity. This work will highlight the computational results and future directions for modeling such complex systems.

[1] M. S. G. Razul, C. J. MacDougall, C. B. Hanna, A. G. Marangoni, F. Peyronel, E. Papp-Szabo and D. A. Pink, Food Funct., 5, (2014) 2501.

[2] C. J. MacDougall, M. S. G. Razul, E. Papp-Szabo, F. Peyronel, C. B. Hanna, A. G. Marangoni and D. A. Pink, Faraday Disc., 158, (2012) 425.

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