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**Digestive Ripening: A Quantitative Thermodynamic Analysis of Stable Nanocrystals** MICHAEL CLARK, SANAT KUMAR, Columbia University, IGAL SZLEIFER, RIKKERT NAP, Northwestern University — Previous studies have shown that stable, monodisperse nanocrystals (NCs) have been produced using strongly binding surfactants, e.g. Au NCs with alkylthiols or Co NCs with oleic acid, to name a few. Through a first-principles theoretical investigation, we develop the full quantitative thermodynamic expression for the state of these surfactant-coated NCs. The general free energy expression allows for the crystal free energy, the surfactant binding energy, surfactant conformational entropy, and the surfactant interactions with other surfactants through excluded volume, solvent depletion, and energetic interactions between surfactant molecules. The energetics of the surfactant chains are treated quantitatively through Single Chain Mean Field theory, which determines the optimal number of grafted surfactants on the surface of an R-sized NC. Then, the size distribution function f(R) is calculated to determine the most favorable NC size and the equilibrium polydispersity. The theoretical conclusions will be compared quantitatively with experimental results. The full thermodynamic expression allows a parametric study of experimentally relevant conditions that govern whether Ostwald ripening vs. digestive ripening vs. dissolution will occur in a given nanocrystal-surfactant system.

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