

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Stable Nanocrystals vs. Ostwald Ripening: A Theoretical Investigation MICHAEL CLARK, SANAT KUMAR, Columbia University, KUMAR GROUP TEAM — Previous studies have shown that stable, monodisperse-sized nanocrystals (NCs) have been produced through the use of 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 determine that these stable sized NCs are in an equilibrium state, and we establish what conditions lead to stable, monodisperse nanocrystals instead of polydisperse nanocrystals undergoing Ostwald ripening. Our results further describe how the equilibrium NC size can be tuned through experimentally adjustable parameters (concentration, temperature, reactant proportions), providing novel concepts for controlling the synthesis of monodisperse nanocrystals. Our theoretical results are compared directly with experimental NC syntheses, providing additional insight into the microscopic properties and dynamics of these stable NC mixtures.

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Date submitted: 22 Nov 2010

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