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Doping colloidal nanocrystals: the role of surfactacts MAO-HUA DU, STEVEN ERWIN, ALEXANDER EFROS, Naval Research Laboratory — The intentional doping of nanocrystals (NCs) with impurity atoms will be critical to their functioning in a variety of technologies. For NCs grown by colloidal synthesis, doping efforts have been far less successful than for their bulk counterparts. We recently proposed a theoretical model that explains this difference [1]. The central idea is that because the temperatures used in colloidal growth are low (250-300 C), thermal equilibrium is never established. Instead, kinetic factors – such as impurity adsorption on the NC surface – play a dominant role in dopant incorporation. Here we consider another kinetic factor known to strongly affect doping in colloidal NCs: the surfactant molecules that are added to passivate the growing NC. We show that the binding strength between the surfactant and dopants in solution strongly affects the dopant sticking coefficient on the NC surfaces, and the dopant solubility in solution. We focus on Mn doping of CdSe NCs, and use first-principles calculations to shed light on the competition between dopant-surface, surfactant-surface, and dopant-surfactant interactions. Our findings are consistent with experimental results for Mn incorporation in CdSe NCs. [1] S.C. Erwin, L. Zu, M.I. Haftel, Al.L. Efros, T.A. Kennedy, and D.J. Norris. Doping semiconductor nanocrystals. Nature **436**, 91 (2005).

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