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Impurity Doping in PbSe Nanocrystals STEVEN ERWIN, Naval Research Laboratory — We recently proposed that impurity doping in colloidally grown nanocrystals is controlled primarily by kinetics, rather than by thermodynamics.[1] In this "trapped dopant" model, the diffusion of an impurity through a nanocrystal is negligible at colloidal growth temperatures. Therefore, an impurity can only be incorporated into a growing nanocrystal if it first adsorbs on the surface and is then overgrown. But this simple surface adsorption process is complicated by a competing process: the binding of the impurity by surfactant molecules, which are used in the growth solution to passivate the nanocrystal and control its growth. Here we use density-functional theory to study the interplay and outcome of these two processes for the doping of PbSe nanocrystals by a variety of candidate impurities (Mn, Cl, In, Cd, Tl) in the presence of several widely used growth surfactants (oleic acid, trioctylphosphine, hexadecylamine).

[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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