

Surface charge formation on ligand – dressed CdSe nanoparticle in hexane

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The charging mechanism of colloidal particles in non-polar solvents by charge control agents or surfactants is not well understood. We employed density functional and density functional tight binding methods to study the formation of charges on bare CdSe nanoparticles of radius 1–5 nm. Thereafter, we explored charge formation on CdSe with different percent surface coverage of adsorbed trioctylphosphine oxide (TOPO) and CdSe + TOPO suspended in hexane. Charge contour plots of the different stages will be presented. The evolution of charge on such suspensions is crucial to comprehend the characteristics of electrophoretic deposition of such nanoparticle suspensions.