

Abstract Submitted  
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**Effects of ligand binding strength and facet coverage on the morphology of nanocrystal superlattices**<sup>1</sup> CLIVE BEALING, RICHARD HENNING, Cornell University — Nanocrystals (NCs) of lead-salt have been proposed for a number of photovoltaic applications. These NCs consist of an inorganic core, in the rock salt structure, whose surface is usually passivated by oleate ligands. The self-assembly of NCs from colloidal solutions into mesoscale superlattices provides a path to materials with tunable electronic, physical and chemical properties that are promising for applications. The self-assembly is controlled by the NC shape and by ligand-mediated interactions between NCs; to understand this, it is necessary to know the effect of the ligands on the surface energies, as well as the relative coverage of the different facets. Our density functional calculations of the binding energies of carboxylic acid-based ligands on PbSe and PbS show that the ligands exhibit a strong energetic preference to particular facets. The results suggest that the transformation of the NC superlattice structure from *fcc* to *bcc* in aged NC assemblies is caused by the preferential detachment of ligands from particular facets, leading to anisotropic ligand coverage. Combined with the experimental results, our calculations present a potential route to greater control over the morphology of the NC superlattice assembly.

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