

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Nanointerfaces in InAs-Sn₂S₆ nanocrystal-ligand networks: atomistic and electronic structure from *first principles*¹ EMILIO SCALISE, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research, GIULIA GALLI, University of Chicago — Semiconducting nanocomposites – consisting of nanocrystals (NCs) embedded in a host matrix – offer exciting prospects for solar energy conversion, light emission and electronic applications. Recent advances in wet chemical techniques allow for the synthesis of NCs, their assembly into superlattices and embedding into a host matrix using only inexpensive solution processing. However, the atomistic details of such composites are poorly understood, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a density functional theory investigation of the interaction of Sn₂S₆ ligands with InAs NCs. Employing a grand canonical approach, we considered a multitude of structures possibly realized at the NC-ligand interface, such as surface termination, reconstructions, passivation, substitution of subsurface atoms, ligand dissociation, NC core-shell formation and the adsorption of the ligands on NCs with different structures. This study provides guidance about the experimental conditions which lead to specific structural motifs and highlights the impact of structural details on the composite’s electronic properties.

¹S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972.

Emilio Scalise
Max-Planck-Institute for Iron Research

Date submitted: 13 Nov 2014

Electronic form version 1.4