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Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles[1] EMILIO SCALISE, STEFAN WIPPERMANN, Max Planck Institute fuer Eisenforschung GmbH, GIULIA GALLI, Institute for Molecular Engineering University of Chicago, DMITRI TALAPIN, Chemistry Department University of Chicago — Colloidal nanocrystals (NCs) are emerging as cost-effective materials offering exciting prospects for solar energy conversion, light emission and electronic applications. Recent experimental advances demonstrate the synthesis of fully inorganic nanocrystal solids from chemical solution processing. The properties of the NC-solids are heavily determined by the NCs surface and their interactions with the host matrix. However, information on the atomistic structure of such composites is hard to obtain, 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 systematic theoretical study of the interaction between InAs and InP NCs with $Sn_2S_6^{4-}$ ligands. Employing a grand canonical ab initio thermodynamic approach we investigate the relative stability of a multitude of configurations possibly realized at the NC-ligand interface. Our study highlights the importance of different structural details and their strong impact on the resulting composite's properties. We show that to obtain a detailed understanding of experimental data it is necessary to take into account complex interfacial structures beyond simplified NC-ligand model interfaces.

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