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Ligand engineering of lead chalcogenide nanoparticle solar cells[1]
MARTON VOROS, Materials Science Division, Argonne National Laboratory, NICHOLAS BRAWAND, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Semiconductor nanoparticles (NP) are promising materials to build cheap and efficient solar cells. One of the key challenges in their utilization for solar energy conversion is the control of ligand-NP interfaces. Recent experiments have shown that by carefully choosing the ligands terminating the NPs, one can tailor electronic and optical absorption properties of NP assemblies, along with their transport properties.[1] By using density functional theory based methods, we investigated how the opto-electronic properties of lead chalcogenide NPs may be tuned by using diverse organic and inorganic ligands. We interpreted experiments, and we showed that an essential prerequisite to avoid detrimental trap states is to ensure charge balance at the ligand-NP interface, possibly with the help of hydrogen treatment. [1] Ryan Crisp et al., Scientific Reports 5, 9945 (2015); Carlo Giansante et al., J. Am. Chem. Soc. 137, 1875 (2015).

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