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Energy Level Alignment for Efficient Carrier Transport in PbS Nanoparticles Capped with Cross-linking Ligand[1] DANYLO ZHEREBETSKYY, MARCUS SCHEELE, Materials Sciences Division, Lawrence Berkeley National Laboratory, DAVID HANIFI, YI LIU, Molecular Foundry, Lawrence Berkeley National Laboratory, PAUL ALIVISATOS, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, COMPUTATIONAL MATERIAL SCIENCE AND NANOP SCIENCE GROUP TEAM, ALIVISATOS GROUP COLLABORATION, YI LIU GROUP COLLABORATION — Arrays of inorganic nanoparticle (NP) can be used for different applications from solar cell to LED. The connection between the NP by organic linker molecule and the resulting carrier transport is a major issue in such applications. We theoretically investigate the electronic coupling between the NP and tetrathiafulvalene-tetraacid (TTFTA) as a function of energy level alignment using multiscale theoretical approach. First, standard DFT calculations are applied to get the geometry of TTFTA on NP surface. Second, the correct band structure is obtained for the molecule and surface from GW formalism including relativistic effects. Third, a long range polarization effect due to the NP dielectric media is included. Fourth, the quantum confinement effect is added to the PbS $1S_h$ and $1S_e$ levels. Finally, charge transport rate between NP through the TTFTA cross-linking molecules is calculated under Marcus theory. The resonant alignment between molecular HOMO and 1Sh state of NP is observed for 9.8 nm NP. The alignment is confirmed experimentally using cyclic voltammetry and ambient pressure X-ray photoelectron spectroscopy.

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