Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Comparison of conventional and unconventional ligand spacers in chalcogenide nanocrystals

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1. Stacking of phthalocyanine molecules

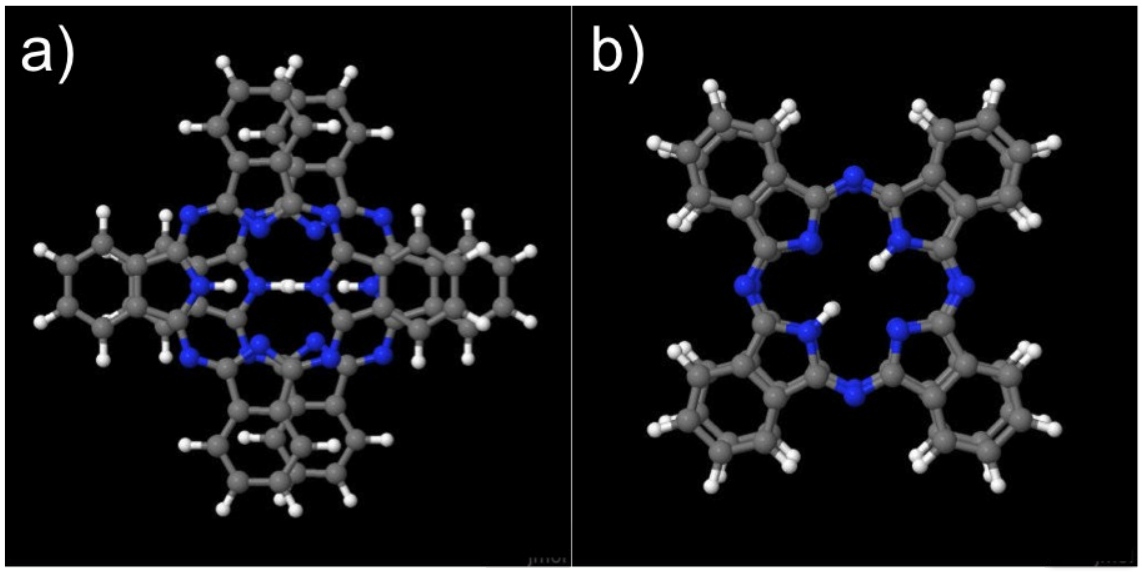

Figure S1. Two phthalocyanine molecules with (a) staggered stacking and (b) AA (eclipsed) stacking. The molecules bind considerably more strongly (by an additional 0.6 eV) in the staggered configuration compared to the eclipsed stacking.

2. Molecular orbitals of phthalocyanine

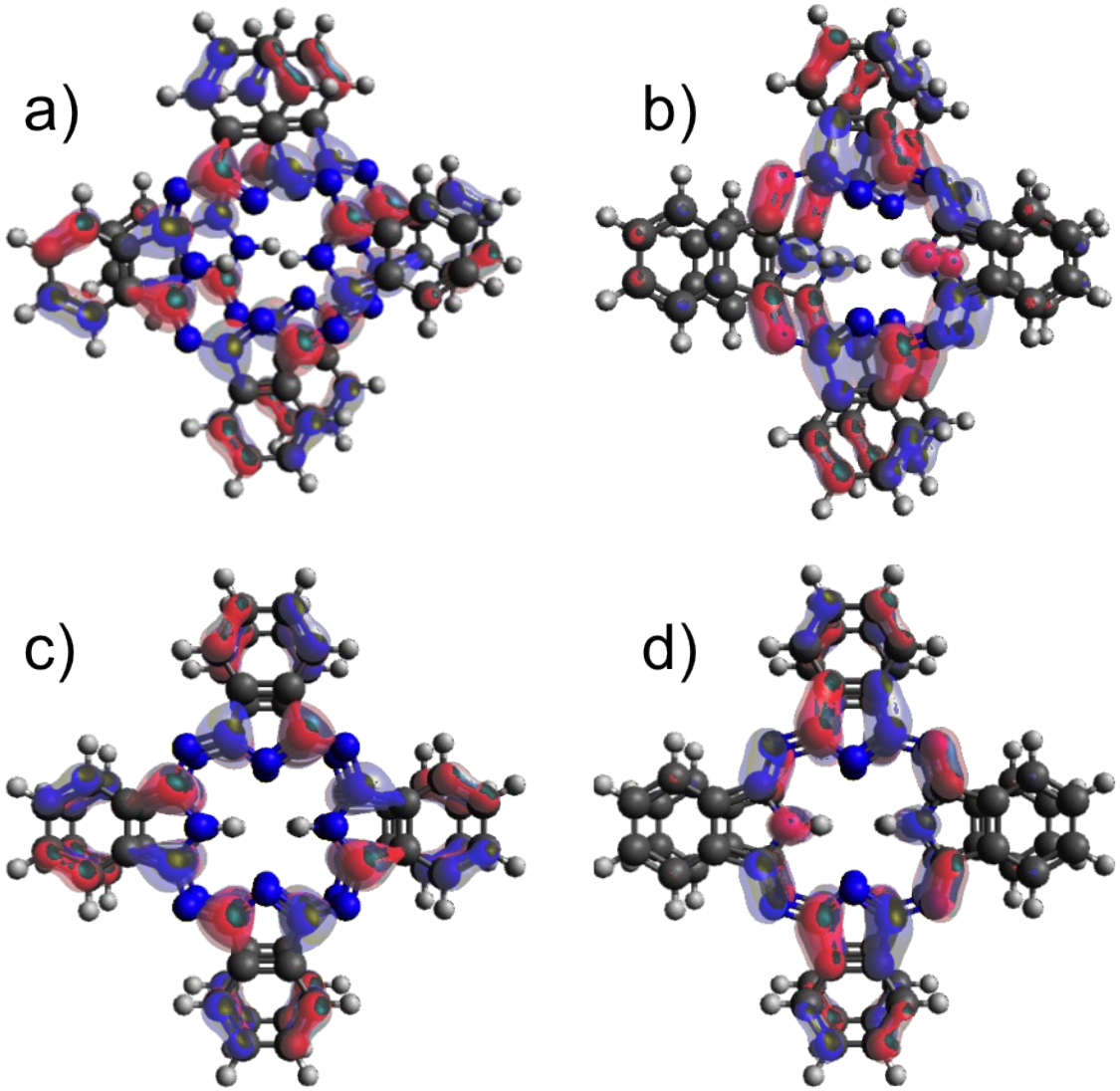

Figure S2. HOMO (left) and LUMO (right) of two phthalocyanine molecules in a staggered (top) and an AA (eclipsed)-stacked configuration (bottom).

3. HOMO-LUMO of Pc-bound NC

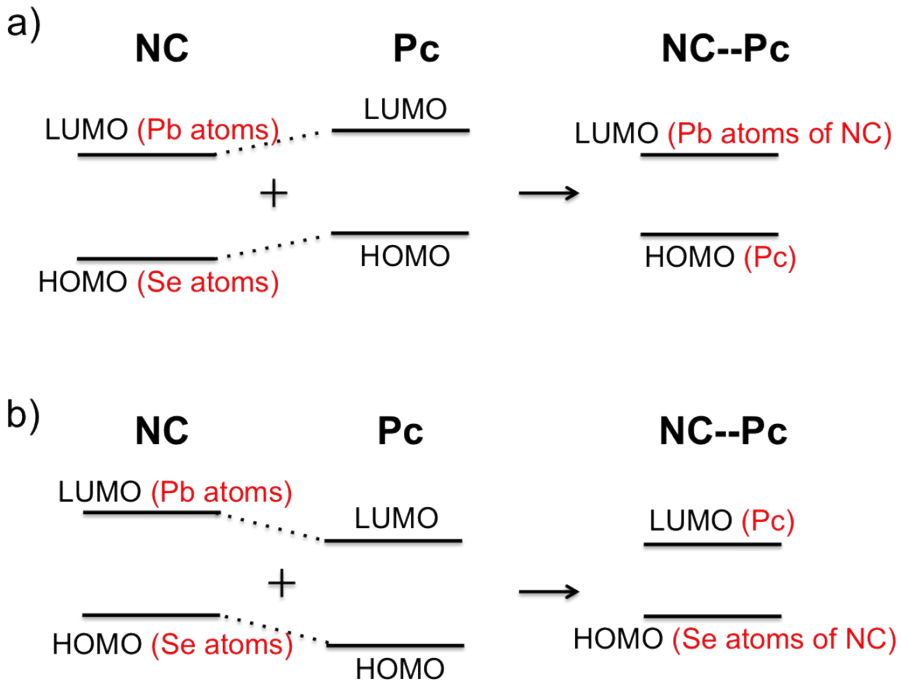

Figure S3. Schematic diagram showing the shift of HOMO and LUMO levels when Pc is bound to either (a) Se-terminated or (b) Pb-terminated facets of the NC. The HOMO and LUMO levels of the bound system in both cases matches the orbital diagrams shown in Figure 5.

4. Molecular orbitals of multiple Pc molecules bound to NC

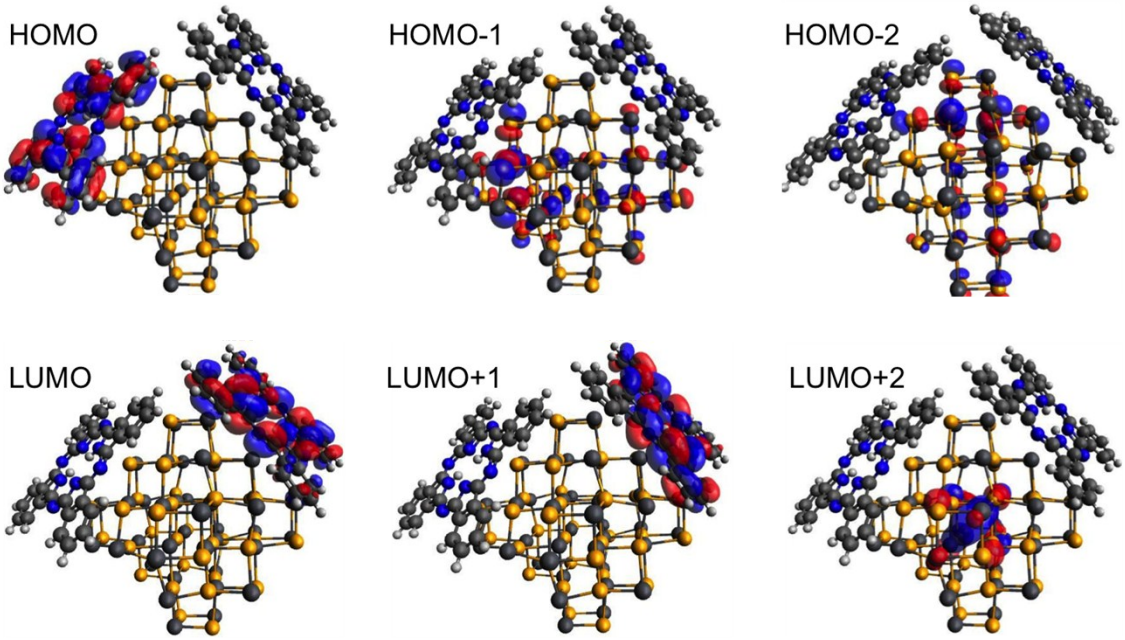

Figure S4. HOMO, HOMO-1, HOMO-2, LUMO, LUMO+1 and LUMO+2 orbitals for a system containing one Pc molecule each on Se-terminated (left-side Pc) and Pb-terminated (right-side Pc) [111] surfaces of a 1.53 nm-dia. PbSe NC. An isovalue of 0.02 is used to plot the orbitals. Atom colors: grey – Pb, yellow – Se for NC, grey – C, blue – N, white – H for Pc.

5. Molecular orbitals of stacked TiOPc

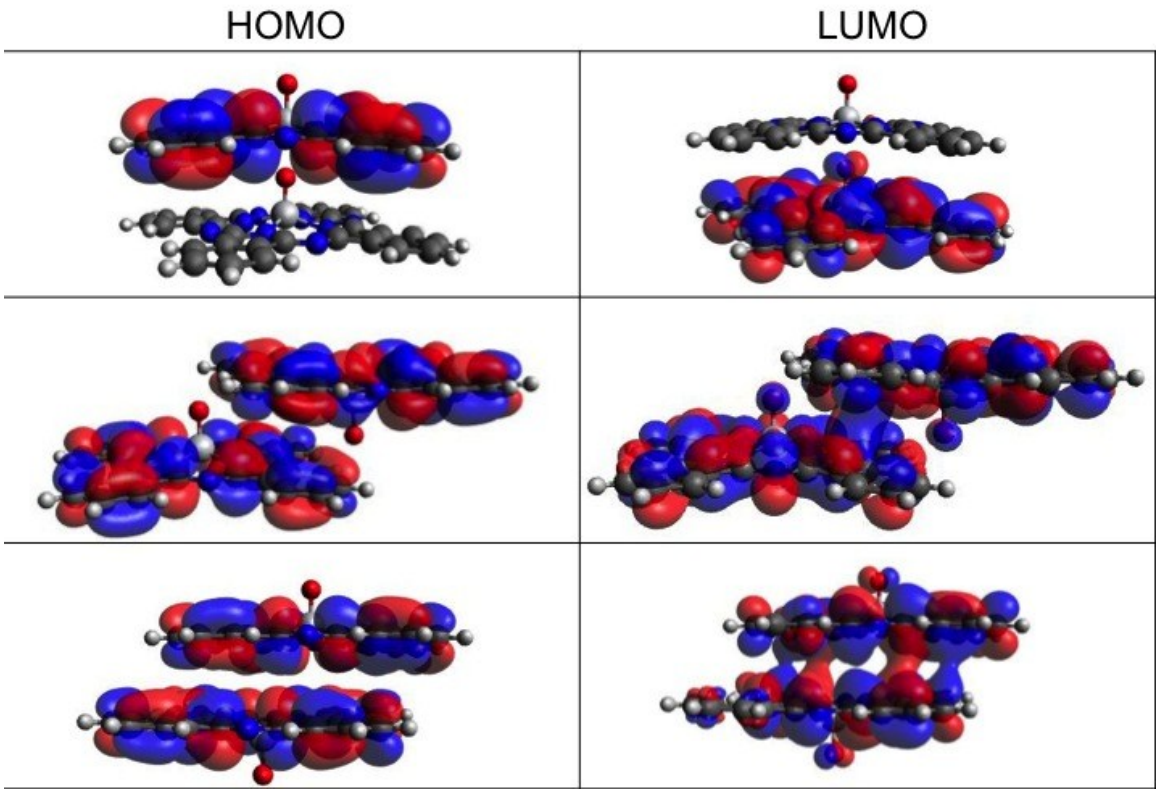

Figure S5. HOMO (left) and LUMO (right) of the three stacking configurations of TiOPc shown in Figure 1.

6. Calculated absorption spectra using TDDFT

The following spectra show extinction coefficient, which is an indicative of the intensity and oscillator strength, which is an indicative of the probability of excitation between two states, as a function of wavelength.

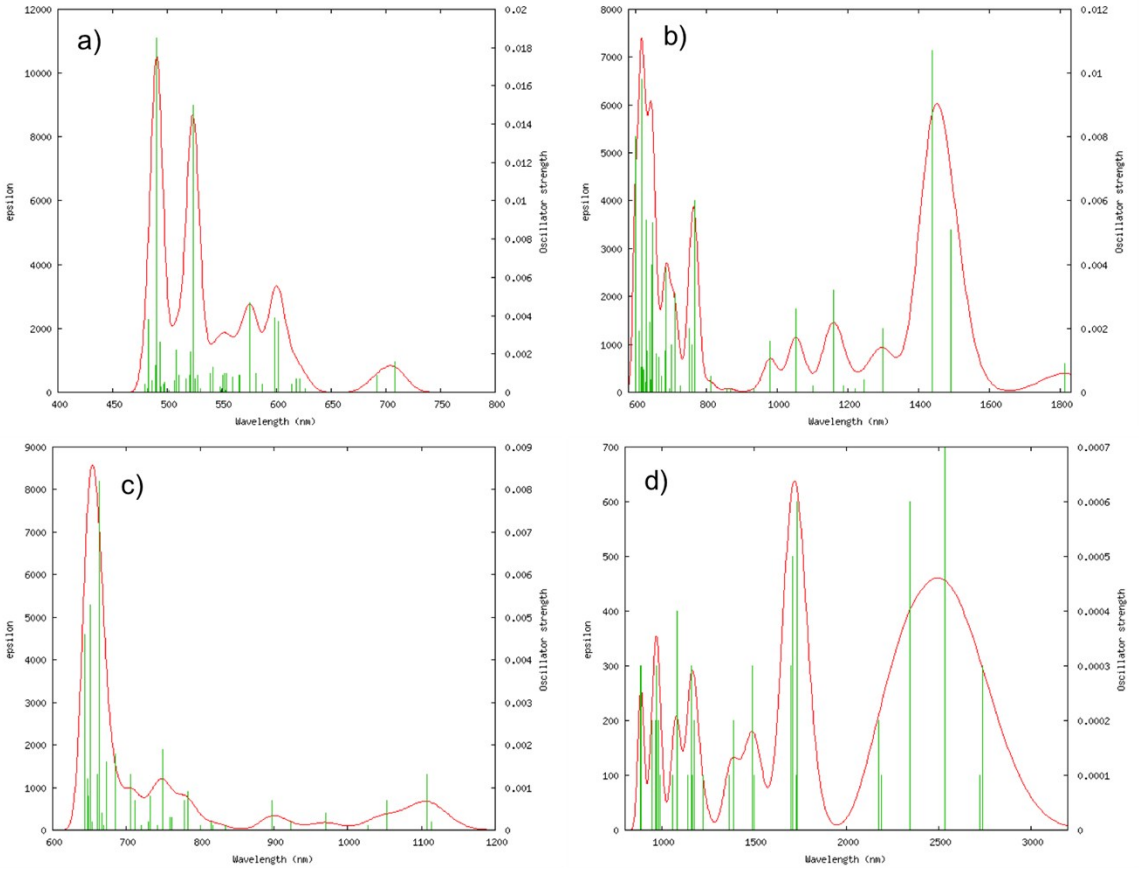

Figure S6. Calculated absorption spectra using TDDFT for the cases of (a) bare NC, (b) EDT-bound NC, (c) Pc bound to a Pb-rich facet of NC and (d) TiOPc bound to a Pb-rich facet of NC.