Electronic Supplementary Information

The Impact of Cation and Anion Pairing in Ionic Salts on Surface Defect Passivation in Cesium Lead Bromide Nanocrystals

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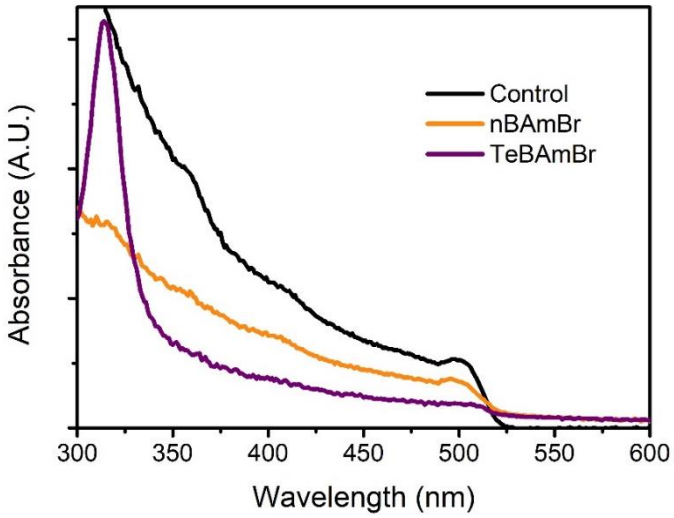

Figure S1. Absorbance spectra of NCs treated with 50 µM of ($nBAm^+$)(Br^-) and ($TeBAm^+$)(Br^-). A decrease in first excitonic peak indicates a general decrease in NC population upon ligand treatment.

Table S1. Averaged PL lifetime values (ns) of control versus various cation – anion pairs.

PL lifetime (ns) Untreated NCs = 1.1	Br^-	DFA^-	BA^-
$OLAm^+$	2.7	2.9	2.5
$TriBAm^+$	2.5	2.1	1.2
$DiBAm^+$	2.7	2.0	1.4

Table S2. Interaction energies of various cation – anion pairs in kJ/mol, computed with B3LYP/ aug-cc-pvtz

Interaction energy (kJ/mol)	Br^-	DFA^-	BA^-
$OLAm^+$	-449	-502	-537
$TriBAm^+$	-402	-427	-459
$DiBAm^+$	-438	-457	-504

Table S3. Interaction energies of various cation – anion pairs in kJ/mol, computed with B3LYP/ aug-cc-pvtz with D3(BJ) dispersion corrections.

Interaction energy (kJ/mol)	Br^-	DFA^-	BA^-
$OLAm^+$	-459	-507	-548
$TriBAm^+$	-426	-454	-482
$DiBAm^+$	-449	-470	-517

Table S4. Interaction energies of various cation – anion pairs in kJ/mol, computed with ωB97X-D/ aug-cc-pvtz.

Interaction energy (kJ/mol)	Br^-	DFA^-	BA^-
$OLAm^+$	-453	-511	-547
$TriBAm^+$	-423	-457	-485
$DiBAm^+$	-444	-474	-518

Table S5. Interaction energies of various cation – anion pairs in kJ/mol, computed with MP2/ aug-cc-pvtz.

Interaction energy (kJ/mol)	Br^-	DFA^-	BA^-
$OLAm^+$	NC[1]	NC	NC
$TriBAm^+$	-456	-467	NC
$DiBAm^+$	-470	-479	-522

[1] Not Calculated (NC) due to memory cost.

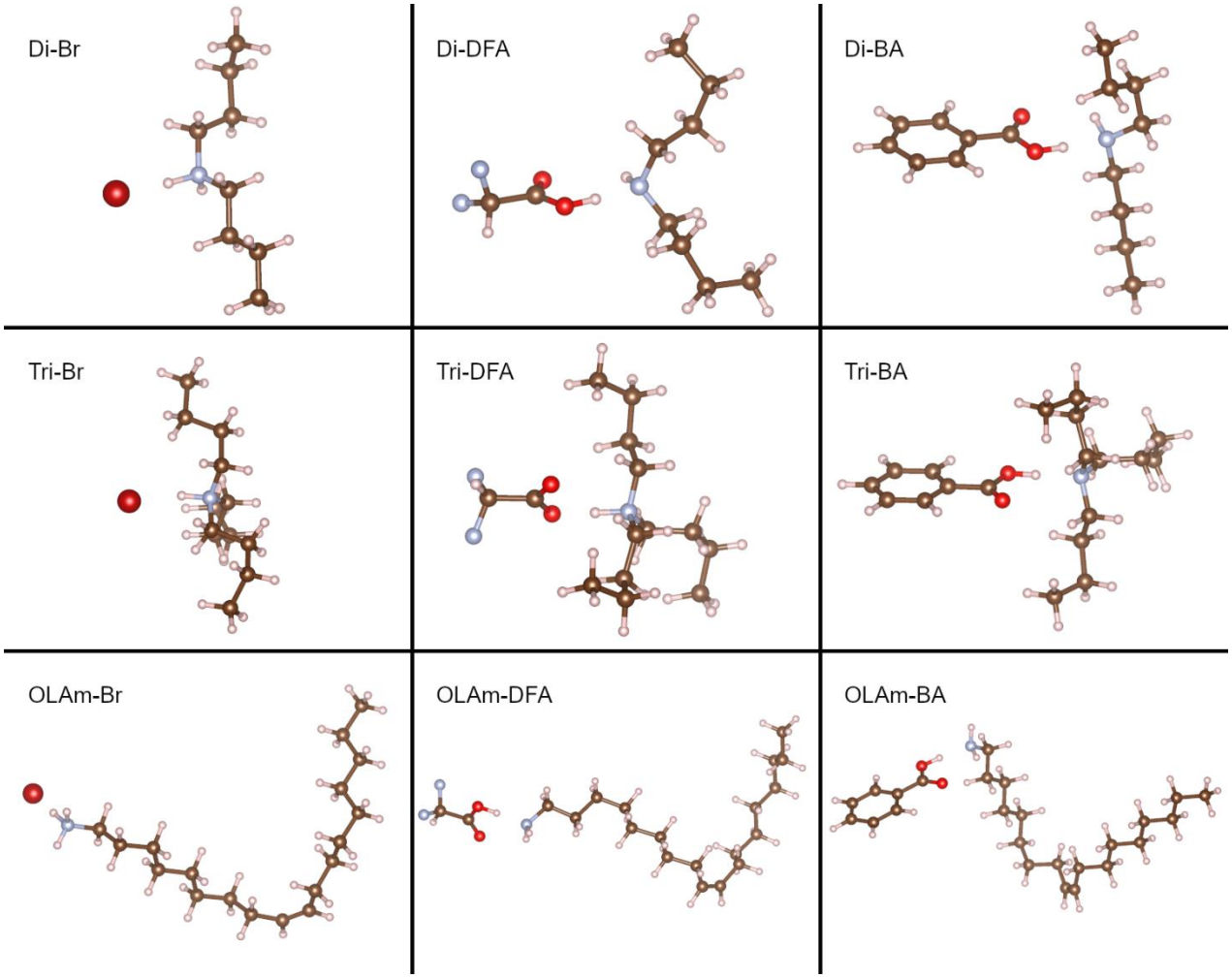

Figure S2. Molecular structures for the B3LYP/aug-cc-pvtz optimized cation – anion pairs. Colors are: C (brown), H (white), O (red), N (light blue), Br (maroon).