

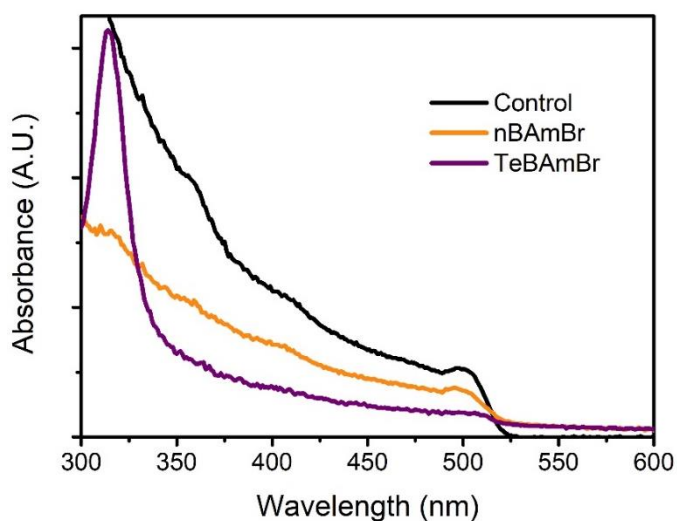
## Electronic Supplementary Information

### 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  $\mu\text{M}$  of  $(\text{nBAm}^+)(\text{Br}^-)$  and  $(\text{TeBAm}^+)(\text{Br}^-)$ . 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	$\text{Br}^-$	$\text{DFA}^-$	$\text{BA}^-$
$\text{OLAm}^+$	2.7	2.9	2.5
$\text{TriBAm}^+$	2.5	2.1	1.2
$\text{DiBAm}^+$	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)	$\text{Br}^-$	$\text{DFA}^-$	$\text{BA}^-$
$\text{OLAm}^+$	-449	-502	-537
$\text{TriBAm}^+$	-402	-427	-459
$\text{DiBAm}^+$	-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 <sup>-</sup>	DFA <sup>-</sup>	BA <sup>-</sup>
OLAm <sup>+</sup>	-459	-507	-548
TriBAm <sup>+</sup>	-426	-454	-482
DiBAm <sup>+</sup>	-449	-470	-517

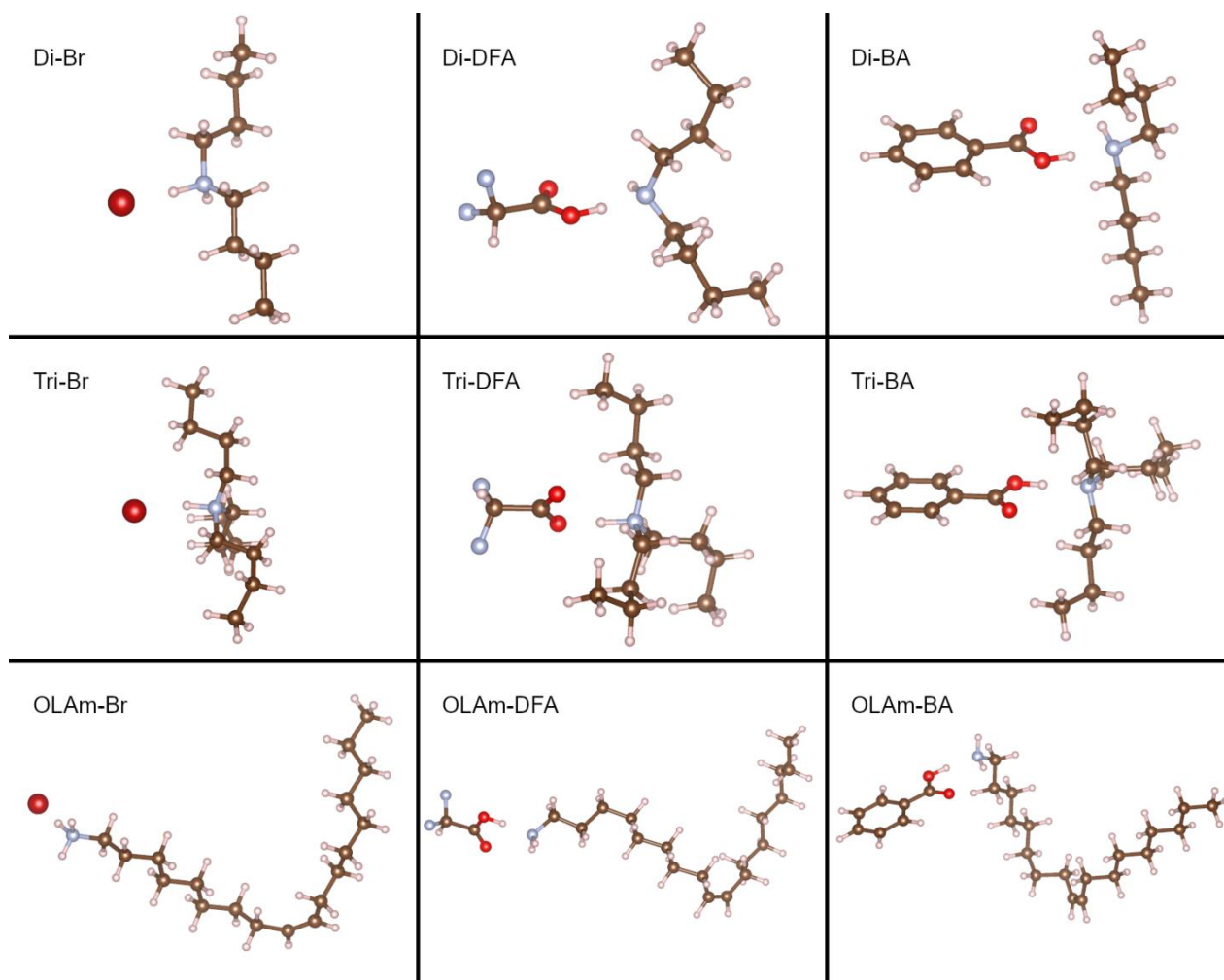
**Table S4.** Interaction energies of various cation – anion pairs in kJ/mol, computed with  $\omega$ B97X-D/ aug-cc-pvtz.

Interaction energy (kJ/mol)	Br <sup>-</sup>	DFA <sup>-</sup>	BA <sup>-</sup>
OLAm <sup>+</sup>	-453	-511	-547
TriBAm <sup>+</sup>	-423	-457	-485
DiBAm <sup>+</sup>	-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 <sup>-</sup>	DFA <sup>-</sup>	BA <sup>-</sup>
OLAm <sup>+</sup>	NC <sup>1</sup>	NC	NC
TriBAm <sup>+</sup>	-456	-467	NC
DiBAm <sup>+</sup>	-470	-479	-522

<sup>1</sup> 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).