Supporting Information

Effects of the methylammonium ion substitutions by 5-ammoniumvaleric acid in lead trihalide perovskite solar cell: A combined experimental and theoretical investigation

Rodrigo Urzúa-Leiva[a], Amir Narymany Shandy[b], Haibing Xie[b], Mónica Lira-Cantú[b]*, Gloria Cárdenas-Jirón[c]*

[a]Instituto de Ciencias Químicas Aplicadas, Facultad de Ingeniería, Universidad Autónoma de Chile, Av. Pedro de Valdivia 425, 7500912, Providencia, Santiago, Chile. [b]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, and the Barcelona Institute of Science and Technology (BIST), Bellaterra E-8193, Spain. [c]Laboratory of Theoretical Chemistry, Faculty of Chemistry and Biology, University of Santiago de Chile (USACH), 9170022, Santiago, Chile

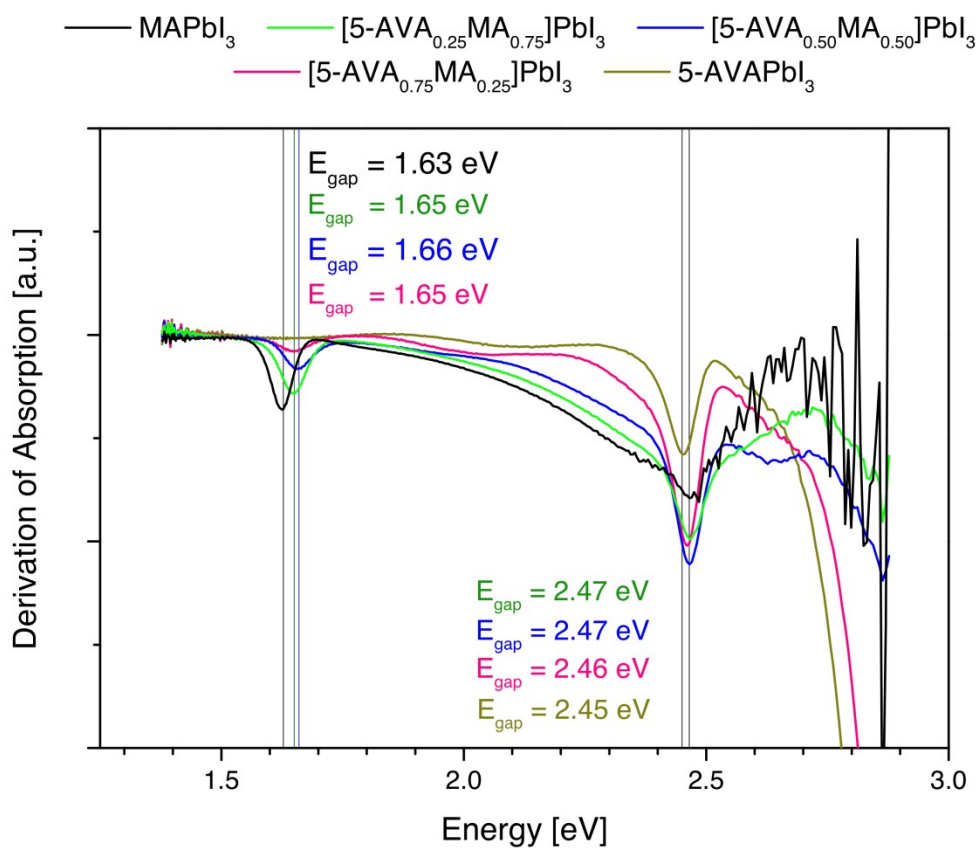


Figure 1. Derivations of the respective absorption spectra (Fig. 4 principal text) to the assignment of bandgaps more precisely and the corresponding absorption peaks. Furthermore, the pure phases of $MAPbI_3$ and 5-$AVAPbI_3$ show only one transition more clearly.

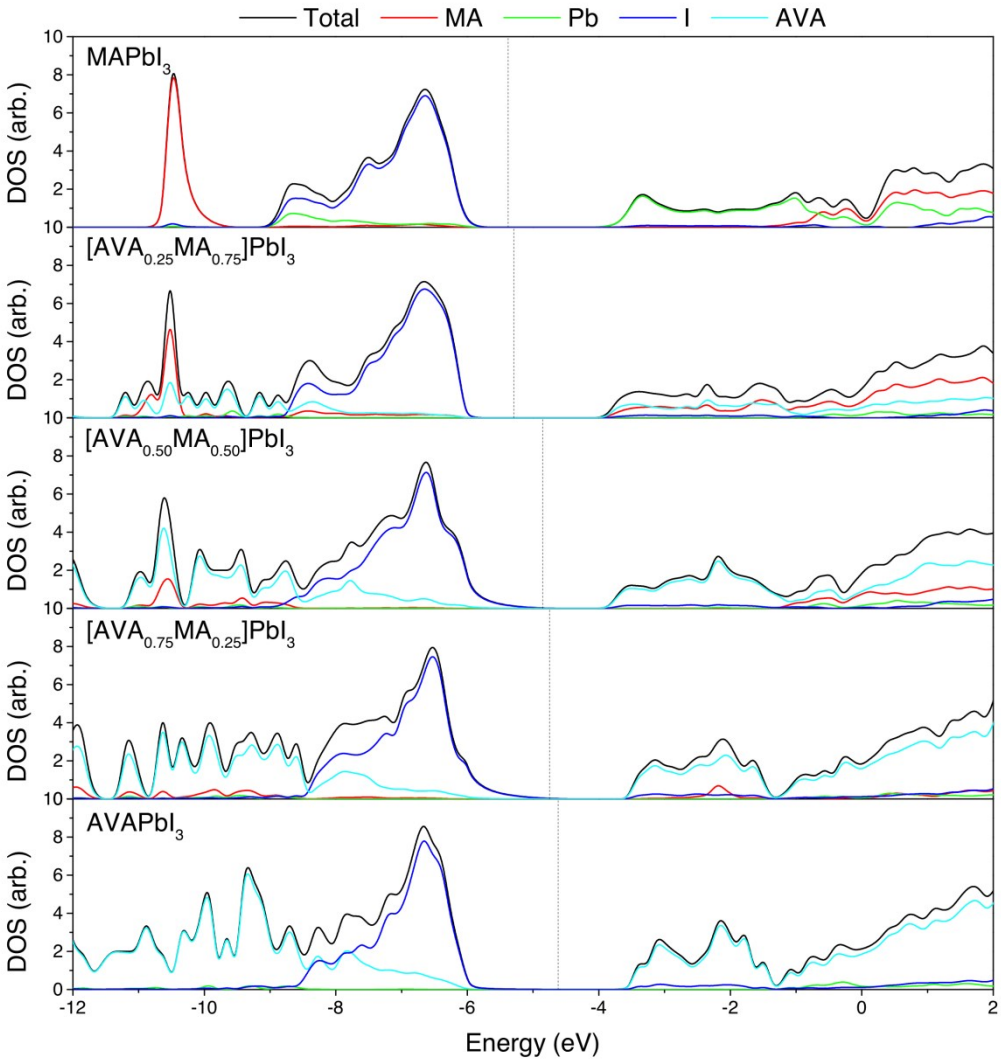


Figure 2. DOS and pDOS calculated at DFT-AE/PBE-D3 level of theory for the five phases of [5-$AVA_{(1-x)}MA_x$]PbI_3 modelled. For a better appreciation, pDOS is separated by atoms (Pb, I) and molecules MA and 5-AVA, as appropriate.

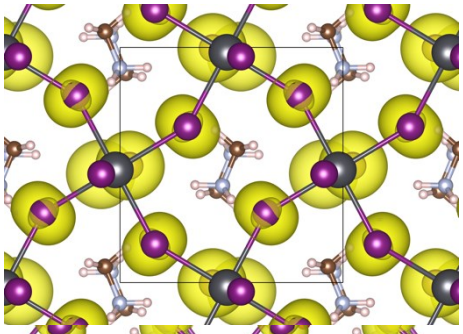
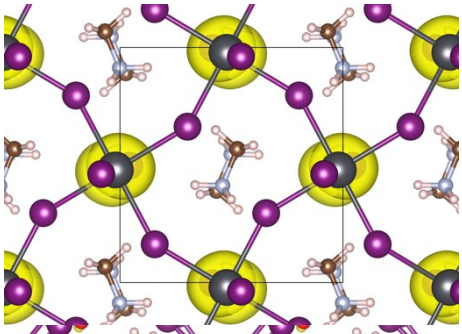
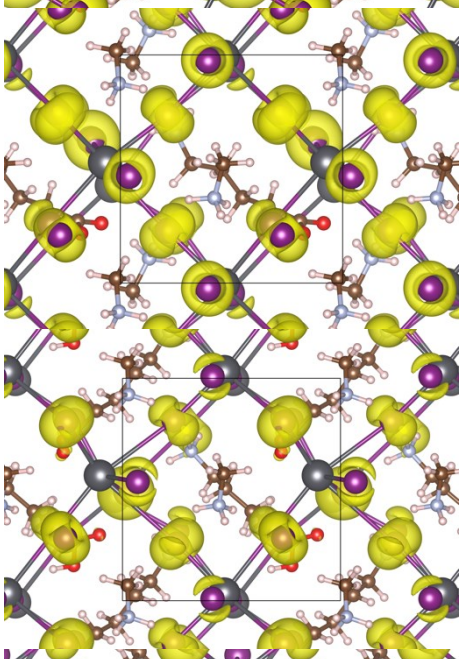
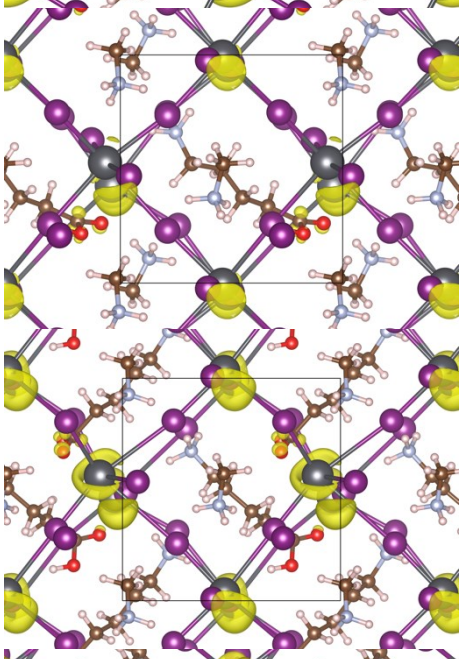
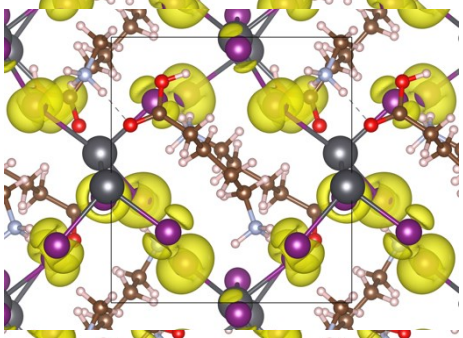
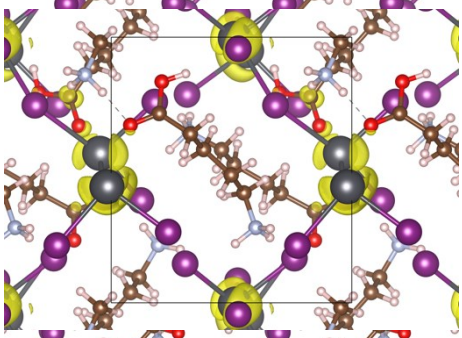
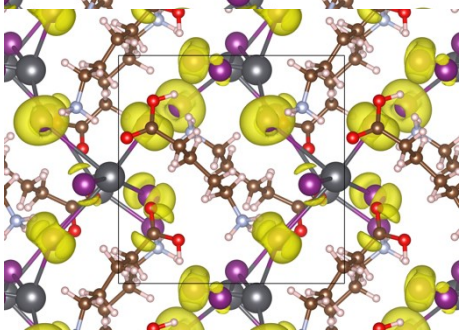
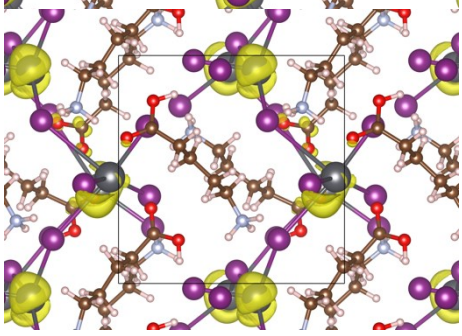
	LDOS Valence Band	LDOS Conduction Band
$MAPbI_3$		
$AVA_{0.25}MA_{0.75}PbI_3$		
$AVA_{0.5}MA_{0.5}PbI_3$		
$AVA_{0.75}MA_{0.25}PbI_3$		
$AVAPbI_3$		

Figure 3. Isosurfaces of the local density of states (LDOS) for the five phases of [5-$AVA_{(1-x)}MA_x$]PbI_3 at ±2 eV of the Fermi level.