Supplemental Material for "Functionality-directed Screening of Pb-free Hybrid Organic-inorganic Perovskites with Desired Intrinsic Photovoltaic Functionalities"

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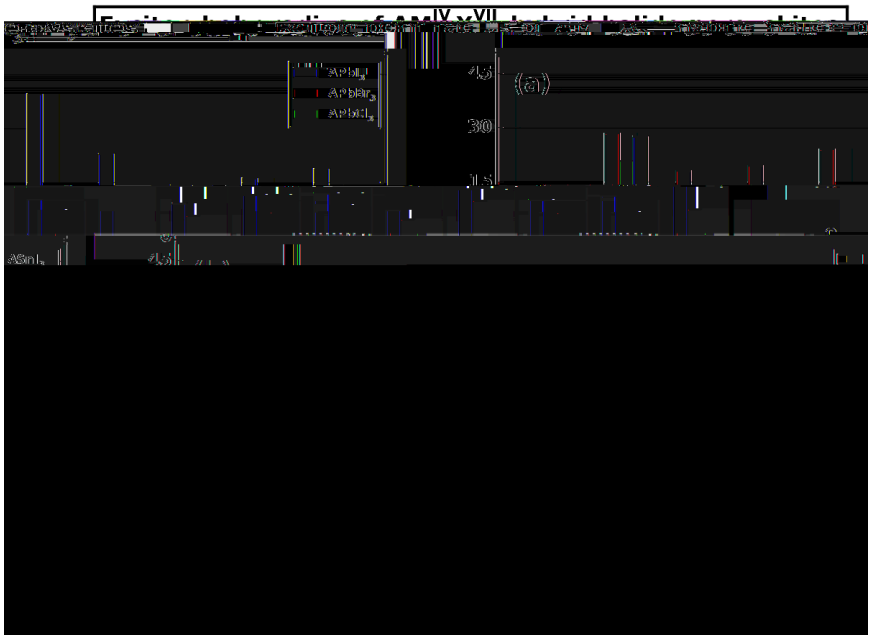

Figure Band structures of the se ected $AM^{IV}X_3^{VII}$ perovs ites having indirect band gaps he va ence band axi u and conduction band ini u are ar ed by red circ es he actua band gaps E_g and direct band gaps E_g^d

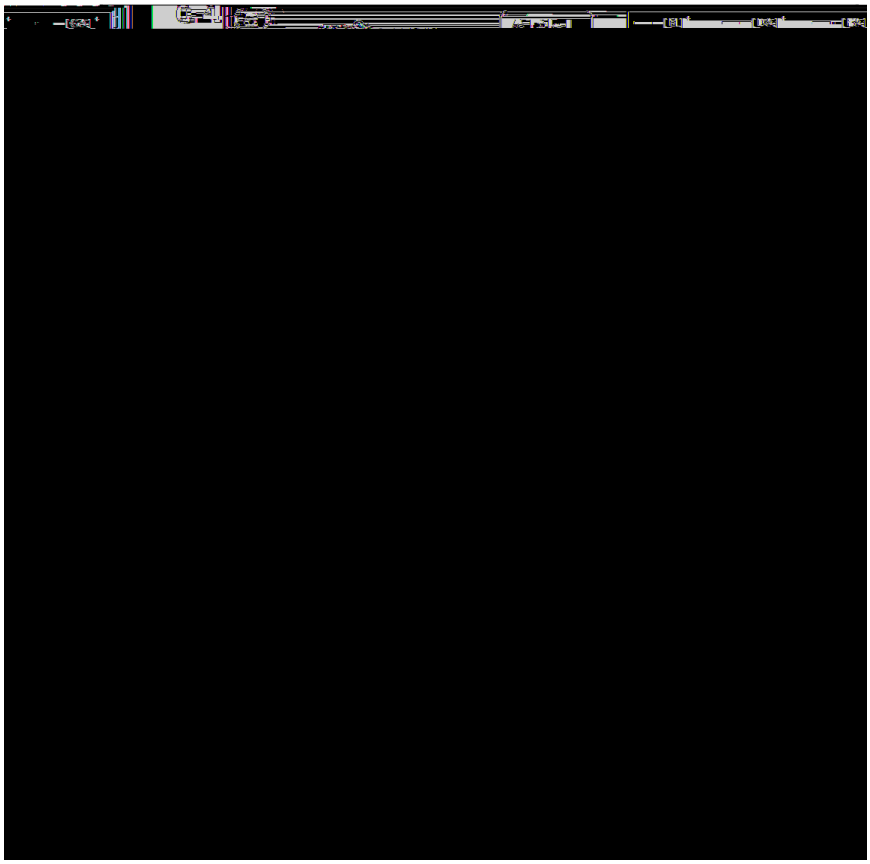

Figure Crysta orbita over ap popu ations COOP of the $AM^{IV}X_3^{VII}$ perovs ites For co parison, the CBM of each ateria is set to energy zero

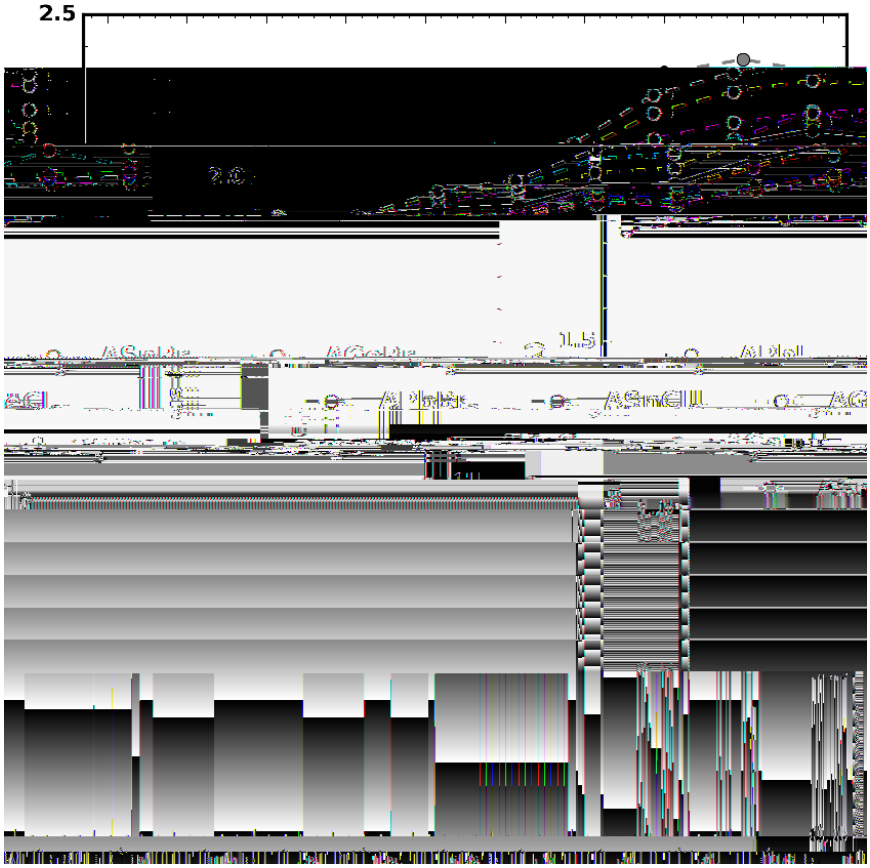

Figure 0 Eva uation of the steric sizes of organic o ecu ar cations within the idea ized so id sphere ode see the Experi enta ection iv

ab e 1 Ca cu ated deco position entha pies H of the candidate $\mathrm{AM}^{IV}\mathrm{X}_3^{VII}$

ab e Ca cu ated direct band gaps E_g^d of the candidate $AM^{IV}X_3^{VII}$ perovs ites he green shading indicates the co pounds passing the current DM $E_g^d <$ e , as we as the DM in ab e ′ he ightb ue shading indicates the co pounds passing on y the current DM

E_g^d e	PbI_3	$PbBr_3$	PbC_3	nI_3	nBr_3	nC_3	GeI_3	$GeBr_3$	GeC_3
[M $^+$									

ab e Ca cu ated exciton binding energies E_B of the candidate $AM^{IV}X_3^{VII}$ perovs ites he green shading indicates the co pounds passing the current DM $E_B <$ e , as we as the DMs in ab es , and he ightb ue shading indicates the co pounds passing on y the current DM

E_B e	PbI_3	$PbBr_3$	PbC_3	nI_3	nBr_3	nC_3	GeI_3	$GeBr_3$	GeC_3
M^+									
Cs^+									
HA^+									
DA^+									
MA^+									
FM^+									
FA^+									
EA^+									
GA^+									
DEA^+									

ab e a_0 Ca cu ated exciton Bohr radii α

ab e Ca cu ated various DMs for the $AM^{IV}X_3^{VII}$ perovs ites containing pseudo ha ogen anions, AM^{IV} $BF_{4\ 3}$ and AM^{IV} $CN_{\ 3}$ with A Cs^{+}, MA^{+}, FA^{+} and M^{IV} Pb^{2+}, n^{2+}

Materia s	H	E_g^d	$^{*}_{e}$	$^{*}_{h}$	E_B e	α_{ex} n
	Co pounds based on $BF_4{}^{-}$					
CsPb $BF_{4\ 3}$						
Cs n $BF_{4\ 3}$						
MAPb $BF_{4\ 3}$						
MA n BF4						
	C pounds based on CN^{-}					
CsPb $CN_{\ 3}$						