Supporting Information for

Rb+ cations enable the change of luminescence properties in Perovskite (RbxCs1-xPbBr3)quantum dots

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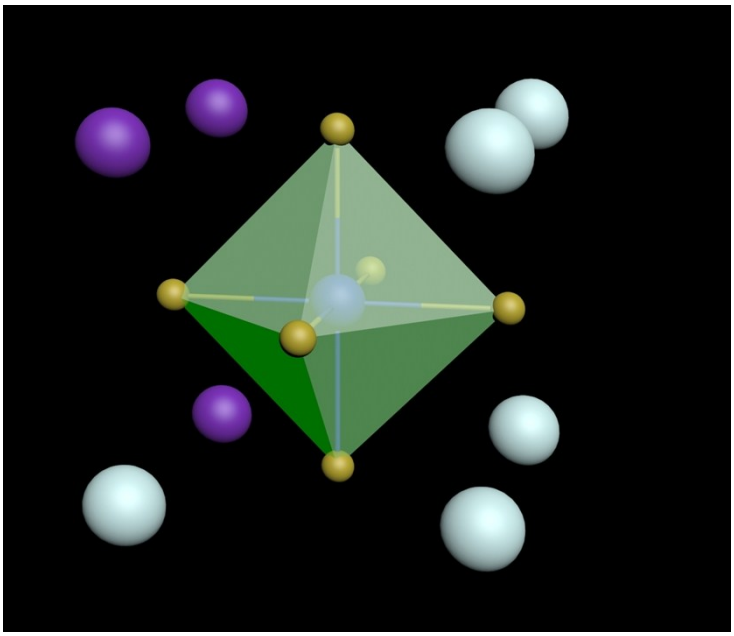


Figure.1s A schematic of the [$PbBr_6$] octahedron and Pb-Br bonds in the unit cell of $Rb_xCs_{1-x}PbBr_3$ with pm-3m space group.

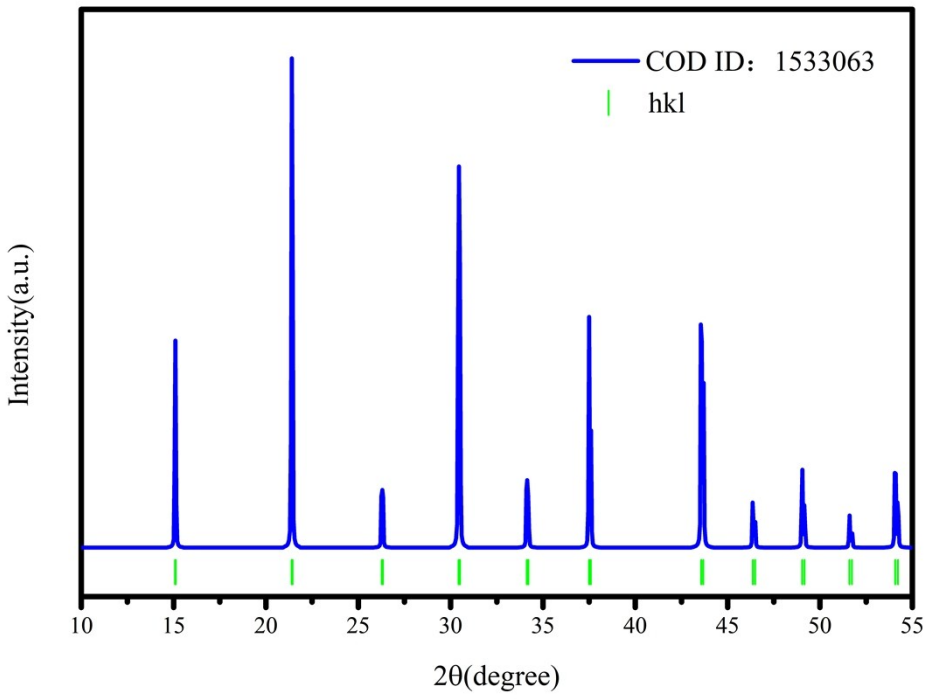
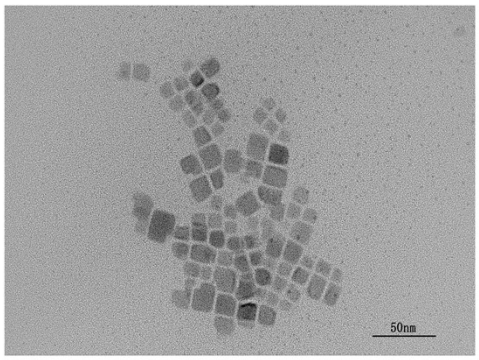
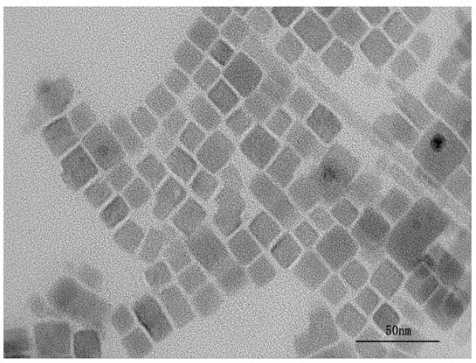


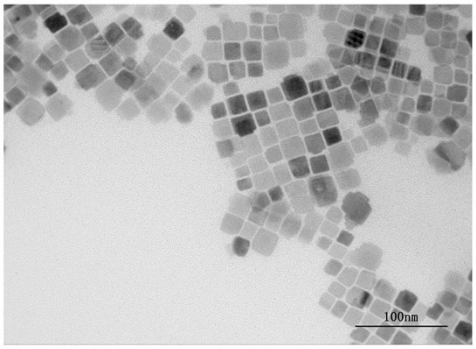
Figure.2s The calculated XRD spectrum of $CsPbBr_3$ with pm-3m space group.



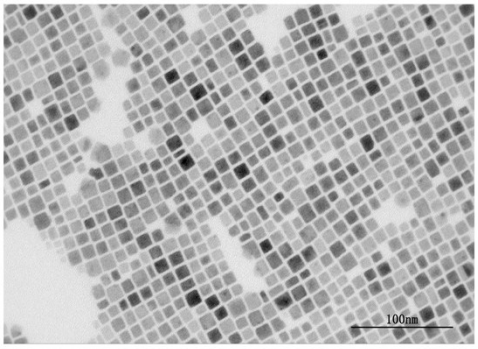
$Rb_{0.75}Cs_{0.25}PbBr_3$



$Rb_{0.5}Cs_{0.5}PbBr_3$



$Rb_{0.25}Cs_{0.75}PbBr_3$



$CsPbBr_3$

Figure.3s The TEM images with different molar concentrations of Rb ions.

Materials Studio (MS) was used to simulate the crystal lattice structure and energy band structure of $Rb_xCs_{1-x}PbBr_3$, which were determined with CASTEP. Cubic $CsPbBr_3$ with pm-3m space group, which corresponds to COD ID (1533063), was used as the lattice structure of the original perovskite. Virtual crystal approximation method was used for the doping of Rb atoms. We modified the Cs atomic lattice atom ratio in 'isMixtureAtom' part to realize random doping. Of course, we also calculated cell units by establishing supercell and replacing the corresponding atoms, and arrived at the same result as with the virtual crystal approximation. Since the latter is a definite location doping structure, the band structure and the density of states were still calculated with the virtual crystal approximation method. When discussing the influence of the bond angle change on the energy band and the electron density distribution, supercell and atom-replacing were used. The geometric structure of $Rb_xCs_{1-x}PbBr_3$ sample was optimized using the generalized gradient approximation (GGA) and Wu and Cohen (WC)[1] function with a cutoff energy of 500 eV. The Brillouin zone was sampled with 12×12×12 Monkhorst and Pack k-points. The lattice parameters were optimized until the forces and total energy converged within 0.01 eV/Å and $5x10^{-6}$eV, respectively. After that, the band structure and density of states were also calculated using the GGA and WC function with the same parameters of lattice optimization.

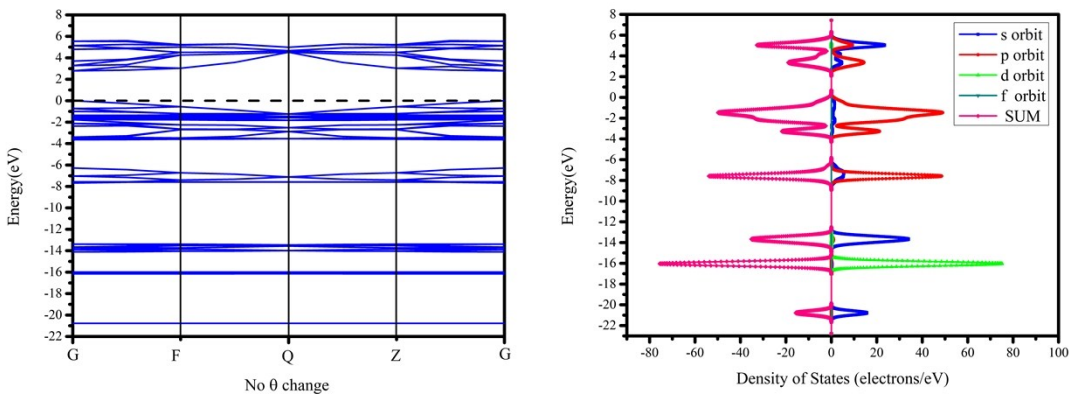


Figure.4s(a) The band structure and DOS of the initial crystal structure.

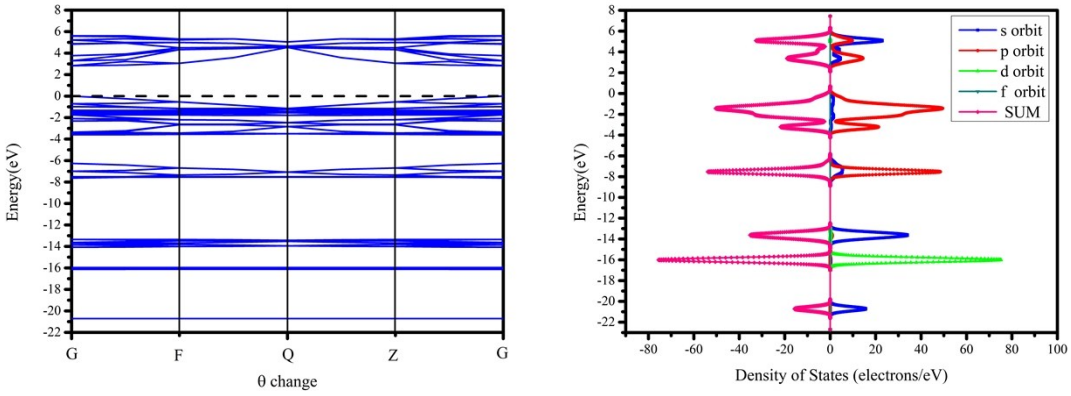


Figure.4s(b) The band structure and DOS of crystal structure with in-plane Pb-Br-Pb bond angle θ change.

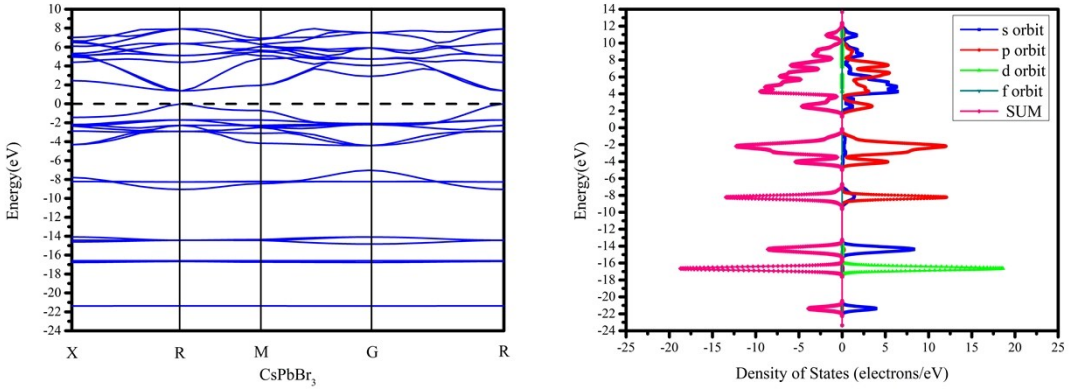


Figure.4s(c) The band structure and DOS of $CsPbBr_3$ crystal structure with pm-3m space group.

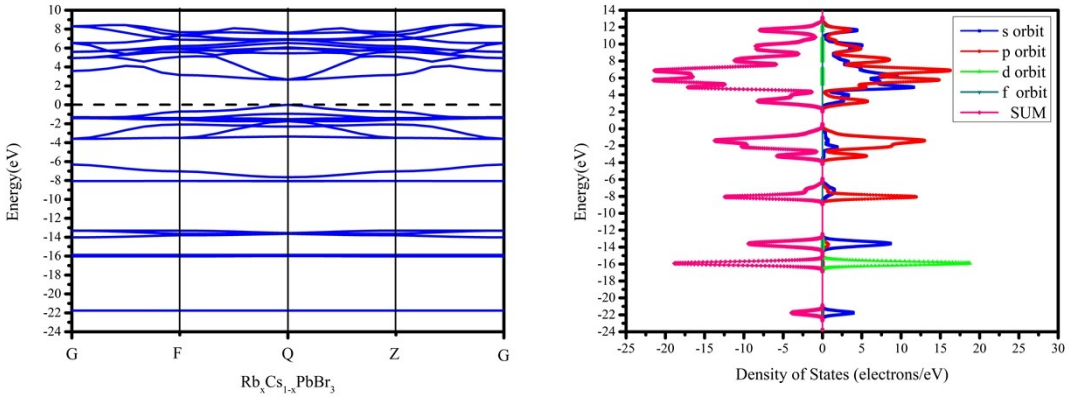


Figure.4s(d) The band structure and DOS of $Rb_xCs_{1-x}PbBr_3$ crystal structure with pm-3m space group.

In order to simply verify that the cation exchange would not appear between the

perovskite quantum dots with different monovalent cations, the photoluminescence properties of mixture were tested and shown in Fig.5s(a) and (b). Only 3nm blue shifting could be observed in Fig.5s(a), and the intensity of luminescence in 435nm was increased slightly. It indicates that it is difficult to achieve cation exchange. In Fig.5s(b), the luminescence position shows red shift from QDs particle growth as a result of Rb-precursors injection at 150℃.

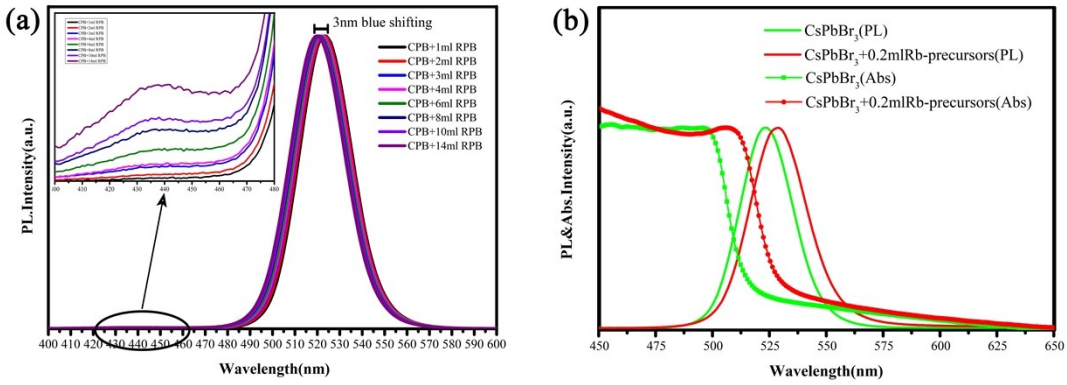


Figure.5s Quantum dots hybrid spectroscopy. (a) The photoluminescence spectra of $CsPbBr_3$ (CPB) mixed with $RbPbBr_3$ (RPB); (b) The photoluminescence spectra of $CsPbBr_3$ mixed with Rb-precursors.

Reference

1. Z. Wu and R. E. Cohen, Physical Review B, 2005, 73, 235116.