Supporting Information for

Photoinduced Localized Hole Delays Nonradiative Electron−Hole Recombination in Cesium–Lead Halide Perovskites: A Time-Domain *Ab Initio* Analysis

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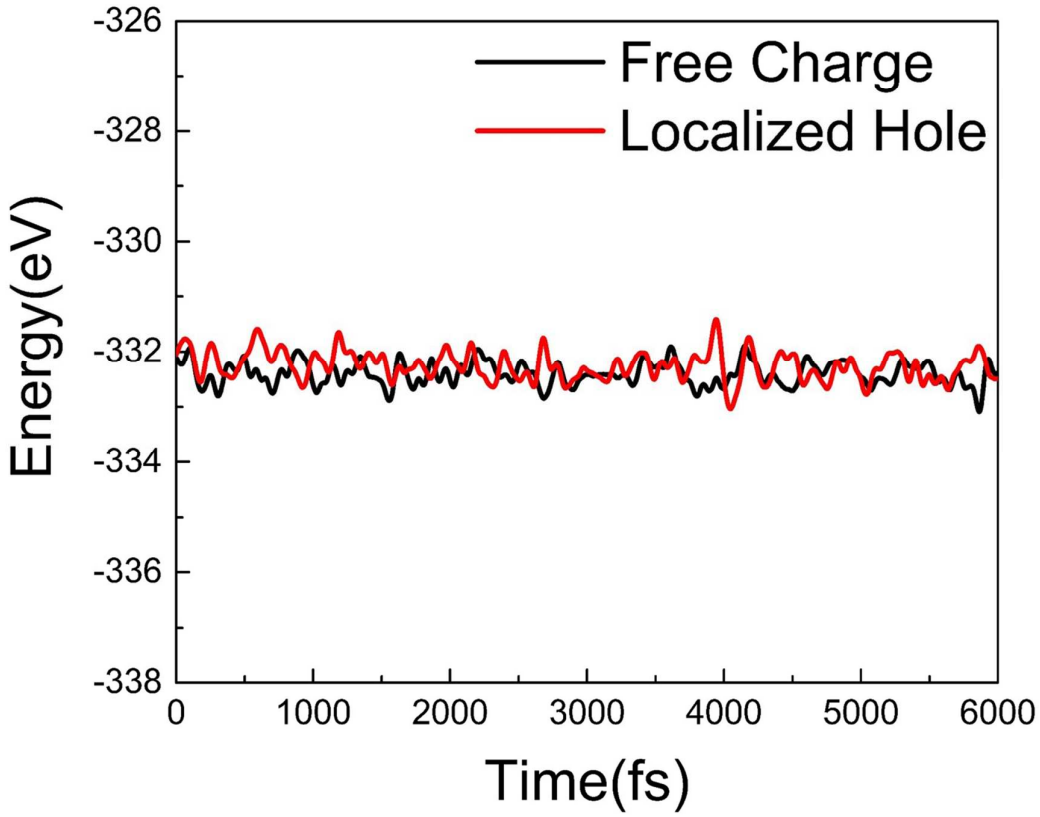

Figure S1. The evolution of total energy for the $CsPbBr_3$ with free charge (black line) and localized hole (red line) for 6 ps MD simulation.

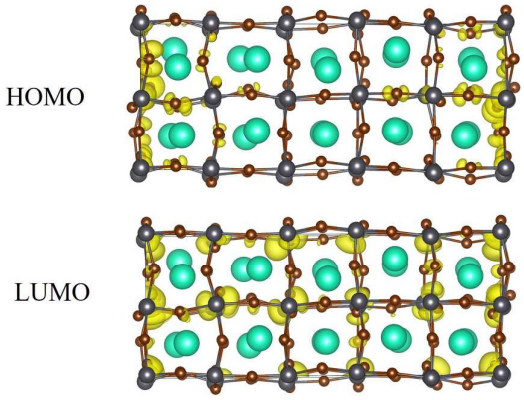

Figure S2. HOMO and LUMO charge densities in polaron structure of (2 × 2 × 5) $CsPbBr_3$ at 300 K. HOMO is localized on the Br and Pb atoms of both edges and the LUMO is delocalized on the entire cell, which is consistent with the charge distribution in Figure 3.

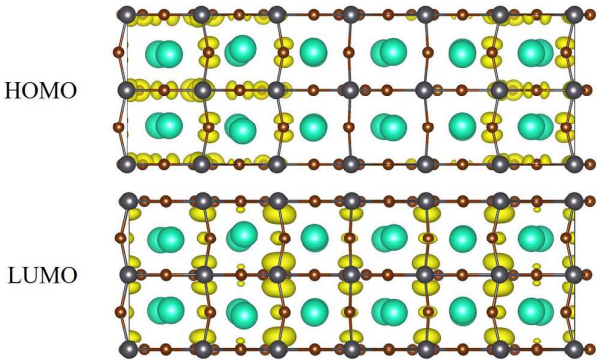

Figure S3. Charge densities of HOMO and LUMO for the (2 × 2 × 6) $CsPbBr_3$ supercell with localized hole obtaind using the optmized geometry at 0 K. The localized hole $CsPbBr_3$ structure is created by changing the angles of Pb-Br-Pb and length of Pb-Br bonds in the (2 × 2 × 6) supercell. The HOMO is localized on partial Br and Pb atoms of the both edges, while the LUMO is delocalized on the whole simulation cell.