Supporting Information for **"Dopants Control Electron-Hole Recombination at Perovskite-TiO_2 Interfaces: *Ab Initio* Time-Domain Study"**

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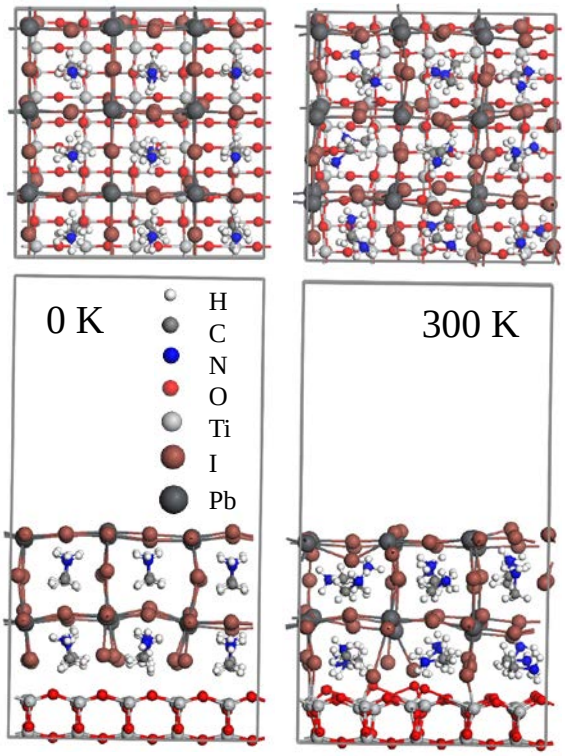

Figure S1. Top and side views of the simulation cell showing geometry of the interface between the2 layer $MAPbI_3$ (100) surface and the TiO_2 anatase (001) surface at 0 K (top panel) and 300 K (bottom panel). Thermal atomic motions alter the geometries and affect the electron donor-acceptor interaction. The geometries at both 0 K and 300 K maintain the major characteristic of the interface between the one layer $MAPbI_3$(100) surface and the TiO_2-anatase(001) surface, Figure 2.

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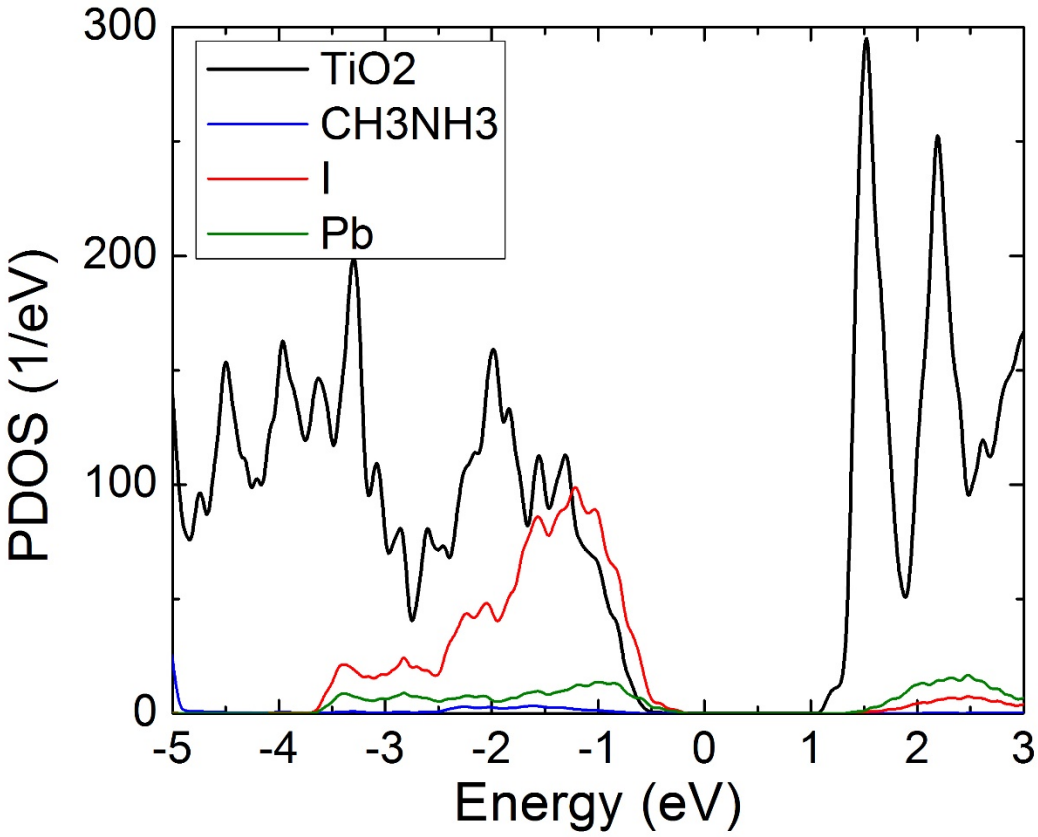

Figure S2. Projected density states (PDOS) of the TiO_2 anatase (001) surface interfaced with the 2 layer $MAPbI_3$ (100) surface at 0 K, Figure S1. The PDOS is split into contribution from TiO_2, CH_3NH_3, I and Pb. The PDOS is nearly identical to the PDOS obtained for the TiO_2 anatase (001) surface interfaced with the 1 layer $MAPbI_3$(100) surface, Figure 1b.

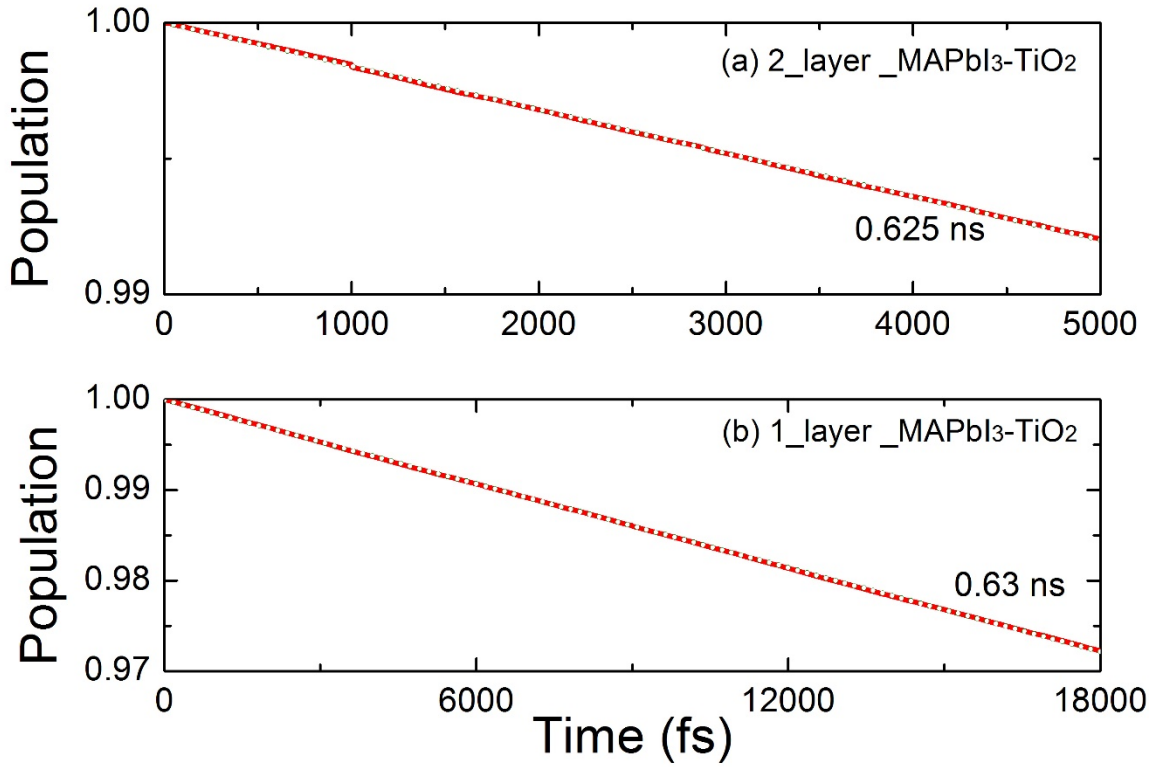

Figure S3. Electron-hole recombination dynamics at the interface between **(a)** the TiO_2-anatase (001) and the 2 layer $MAPbI_3$(100) surface, and **(b)** the TiO_2-anatase (001) surface and the 1 layer $MAPbI_3$(100) surface. The circles are linear fits. Both time scales agree well with the result obtained for the 1 layer system over a shorter time interval, Figure 7, demonstrating that the 1 layer $MAPbI_3$(100)/TiO_2-anatase(001) model is capable of describing the interfacial electron-hole recombination dynamics.