

Supporting Information for

## Computational Study of Ternary Devices: Highly Stable, Low Cost and Efficient Planar Perovskite Solar Cells

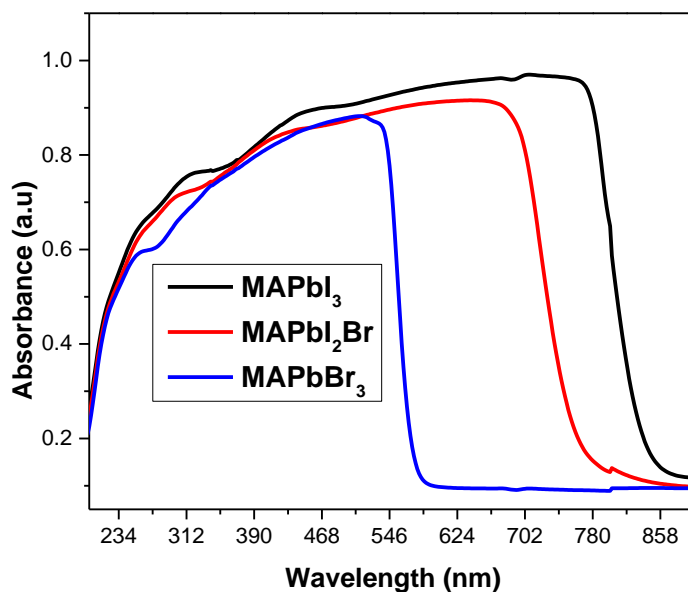
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### Supplementary Figure and Table



**Fig. S1** Absorbance spectra of the MAPbI<sub>3</sub>, MAPbI<sub>2</sub>Br and MAPbBr<sub>3</sub> materials

**Table S1** Basic parameters for thin defect layers at the interfaces of ZnO/perovskite and Cu:NiO<sub>x</sub>/perovskite

<b>Parameters and units</b>	<b>ZnO/perovskite</b>	<b>Cu:NiO<sub>x</sub>/perovskite</b>
Dielectric constant	30	11
Band gap (eV)	1.5	3.6
Electron affinity (eV)	3.93	1.46
Thickness (nm)	2	2
Electron and hole mobility(cm <sup>2</sup> /V/s)	50, 50	0.5, 0.5
Acceptor concentration (cm <sup>-3</sup> )	2.14×10 <sup>17</sup>	1.4×10 <sup>20</sup>
Donor concentration (cm <sup>-3</sup> )	0	0
Effective conduction and density (cm <sup>-3</sup> )	2.5×10 <sup>20</sup>	2×10 <sup>17</sup>
Effective valence band density (cm <sup>-3</sup> )	2.5×10 <sup>20</sup>	1.1×10 <sup>19</sup>
Characteristic energy for donor and acceptor-like tails (eV)	0.015, 0.015	0.01, 0.01
Band tail density of states (1/cm <sup>3</sup> /eV)	1×10 <sup>14</sup>	1×10 <sup>14</sup>
Capture cross section for electrons and holes in donor tail states (cm <sup>2</sup> )	1×10 <sup>-15</sup> , 1×10 <sup>-17</sup>	1×10 <sup>-15</sup> , 1×10 <sup>-17</sup>
Capture cross section for electrons and holes in acceptor tail states (cm <sup>2</sup> )	1×10 <sup>-17</sup> , 1×10 <sup>-15</sup>	1×10 <sup>-17</sup> , 1×10 <sup>-15</sup>
Switch-over energy (eV)	0.7	0.8
Density of mid-gap acceptor and donor-like states (cm <sup>-3</sup> eV <sup>-1</sup> )	1×10 <sup>16</sup> to 1×10 <sup>19</sup>	1×10 <sup>17</sup> to 1×10 <sup>19</sup>
Capture cross section of electrons and holes in donor mid-gap states (cm <sup>2</sup> )	1×10 <sup>-17</sup> , 1×10 <sup>-18</sup>	1×10 <sup>-16</sup> , 1×10 <sup>-17</sup>
Capture cross section of electrons and holes in acceptor mid-gap states (cm <sup>2</sup> )	1×10 <sup>-18</sup> , 1×10 <sup>-17</sup>	1×10 <sup>-17</sup> , 1×10 <sup>-16</sup>