Area: Semiconductor device modeling and simulation

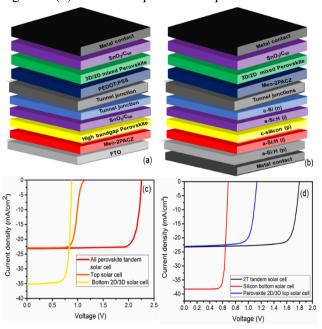
Effect of 2D perovskite layer in all-perovskite and perovskite/silicon tandem solar cells.

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In a multijunction (Tandem) solar cell the quality of surface and interfaces played important role in determining its efficiency and stability. In perovskite-based solar cells, the application of 2D perovskite material on top of the 3D perovskite absorber layer is widely investigated. Here we have simulated and studied the performance of 2D perovskite in perovskite/perovskite and perovskite/silicon tandem solar cells. The effect of various 2D perovskite materials with their layer thickness and interfacial energy band offsets are studied extensively. The 2D perovskite layer was employed in the low bandgap sub-cell of all perovskite TSC and high band gap sub-cell of perovskite/silicon TSC as shown below in Figure 1 (a) and Figure 1 (b). The JV response of all perovskite 2T and perovskite/silicon tandem is shown below in Figure



1 (c) and Figure 1 (d) receptively. In all perovskite tandem solar cell, the absorber layers were chosen as $MA_vFA1_{-v}Sn_{1-v}Pb_vI_3$ (700 nm) bandgap 1.2 eV and FA_vCs_{1-v}PbI_xBr_{1-x} (450 nm) bandgap 1.8 eV, while triple cation perovskite layer (450 nm) with bandgap 1.67 eV was chosen as the absorber layer of top cell in perovskite silicon tandem solar cell. The thickness of c-Si absorber layer was kept at 180 µm. Meo-2PACZ and PEDOT:PSS were simulated as the hole transporting layer for the top and the bottom solar cell respectively. Dual electron transport layer SnO2 and C60 were selected for the electron transport layer. For the perfect addition of open circuit voltage, an ideal tunnel recombination junction was assumed. Tandem solar cells were series-connected using a script file in SCAPS-1D software.

Figure 1 (a): Device schematic of all perovskite tandem. (b): Device schematic of perovskite/silicon tandem. (c): JV response of top, bottom, and all perovskite tandem (d): JV response of top, bottom, and perovskite/silicon tandem.

The highest efficiency of the tandem solar cell was observed at 20 nm of 2D perovskite layer thickness. Interface defect density was studied to mimic the surface passivation impact of the 2D perovskite layer on top of 3D perovskite layer. The charge carrier lifetime varied from 1 μ s to 1 ns upon changing the surface defect density from 10^{14} /cm³ to 10^{17} /cm³ at surface recombination velocity $S_N = S_P = 10^7$ cm/s. A higher photocurrent density and higher open circuit voltage was observed in all perovskite and perovskite/silicon tandem solar cells with the variation of surface charge carrier lifetime from 1 ns to 1 μ s. The improvement was observed due to the surface passivation effect of 2D perovskite on top of the 3D perovskite absorber layer. With the incorporation of 2D perovskite layer, PCE above 30% was observed in all perovskite and perovskite/silicon tandem solar cells.