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First principles modeling of perovskite solar cells based on TiO_2 and Al_2O_3: Stability and Interfacial Electronic Structure

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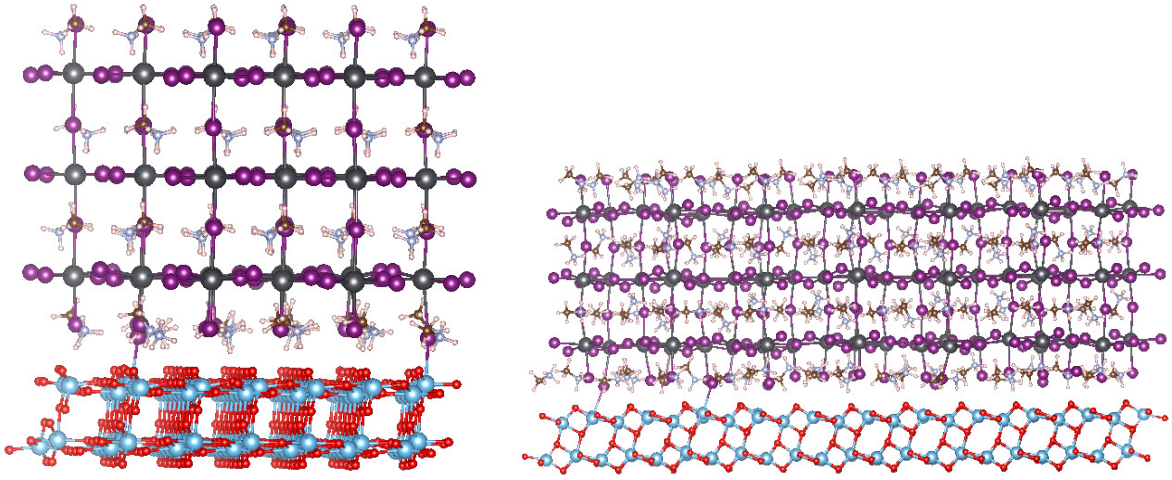

Figure 1: Optimized geometrical structures of the MAPI (110) and (001) on TiO_2. Left:(001) and right (110).

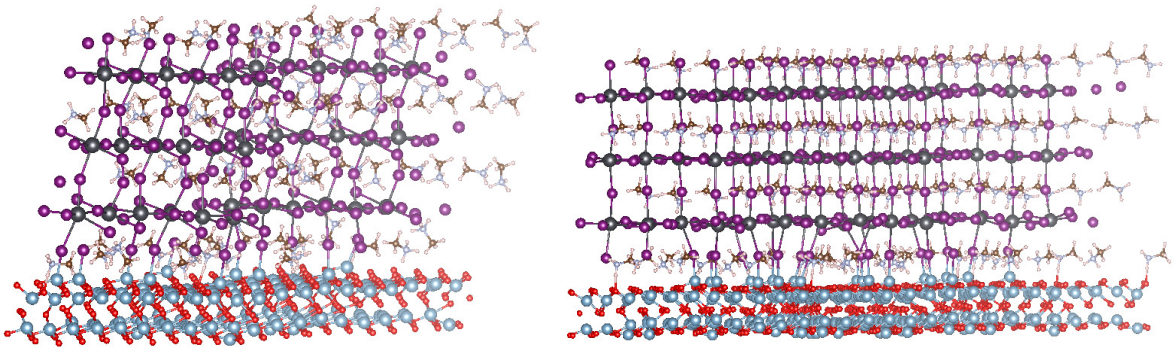

Figure 2: Optimized geometrical structures of the (110) and (001) surface slabs for the MAPbI3 perovskites on α-alumina. Left:(110) and right (001).

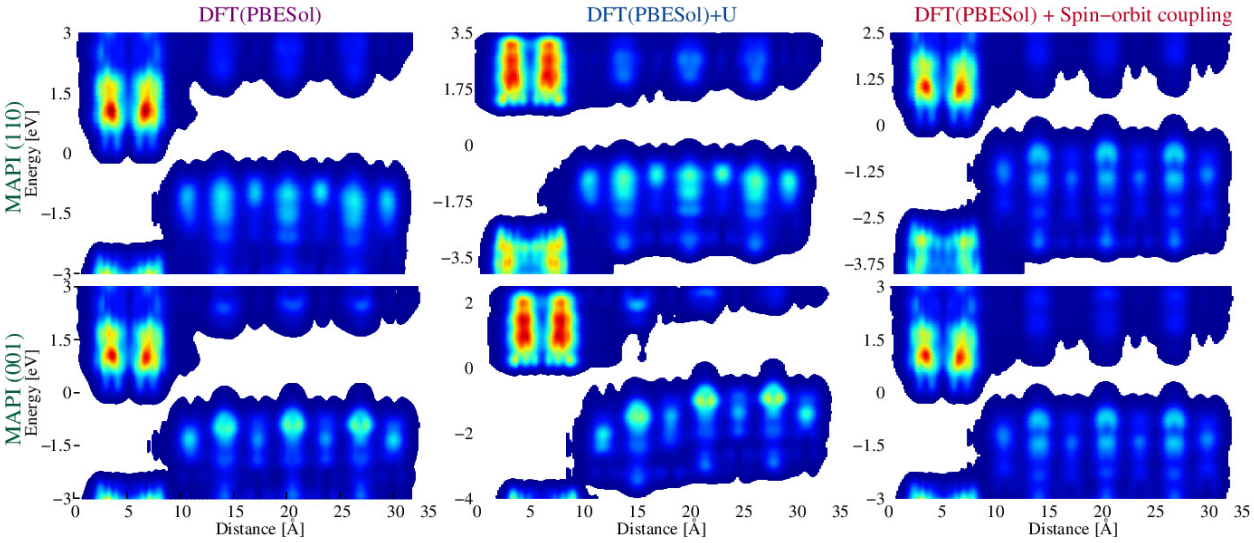

Figure 3: Integrated LDOS for the MAPI (110) and (001) on TiO_2 from different type of electronic structure calculations. U in DFT+U calculations is set to equal nine to correct the bandap of titania.

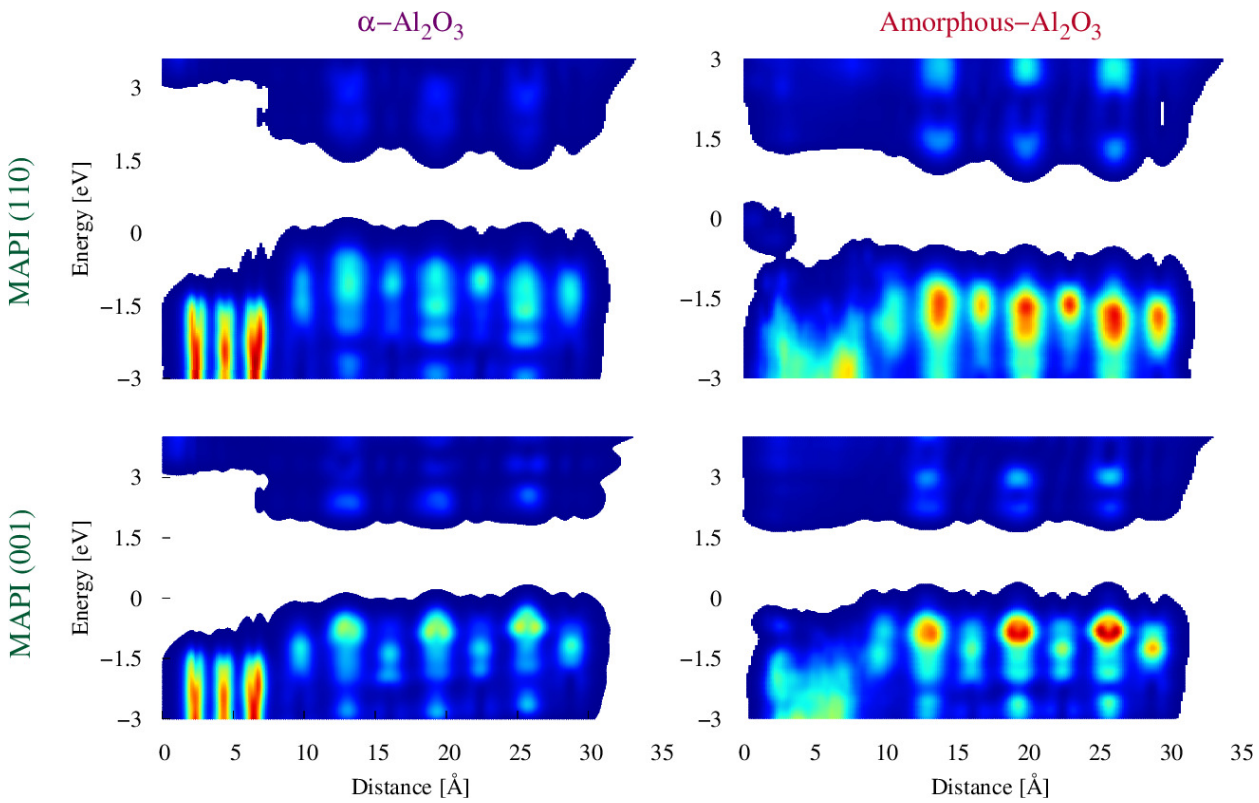

Figure 4: Integrated LDOS for the MAPI (110) and (001) on Al_2O_3 (α-phase and amorphous) from DFT calculations (PBESol, spin-orbit interaction via scaler relativistic treatment).