SUPPORTING INFORMATION TO

Interfacial electronic features in methyl-ammonium lead iodide and p-type oxide heterostructures: new insights for inverted perovskite solar cells

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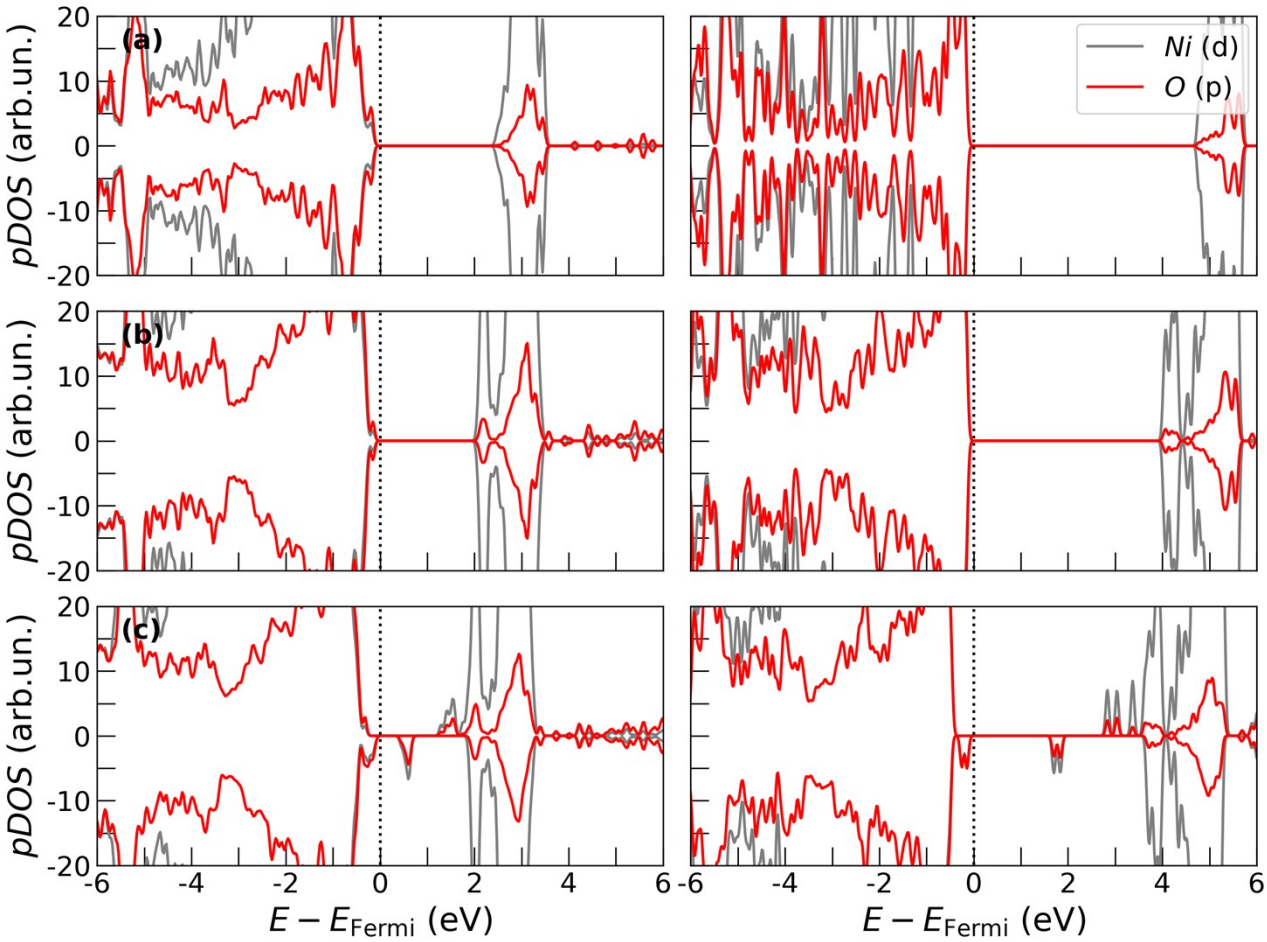

Figure S1. Spin-resolved atom-angular momentum-projected densities of states (pDOS) at PBE+U (left side) and HSE (right side) level of theory calculated for the bulk NiO (panel a), for the NiO pristine slab (panel b) and for the defective NiO:VNi slab (panel c).

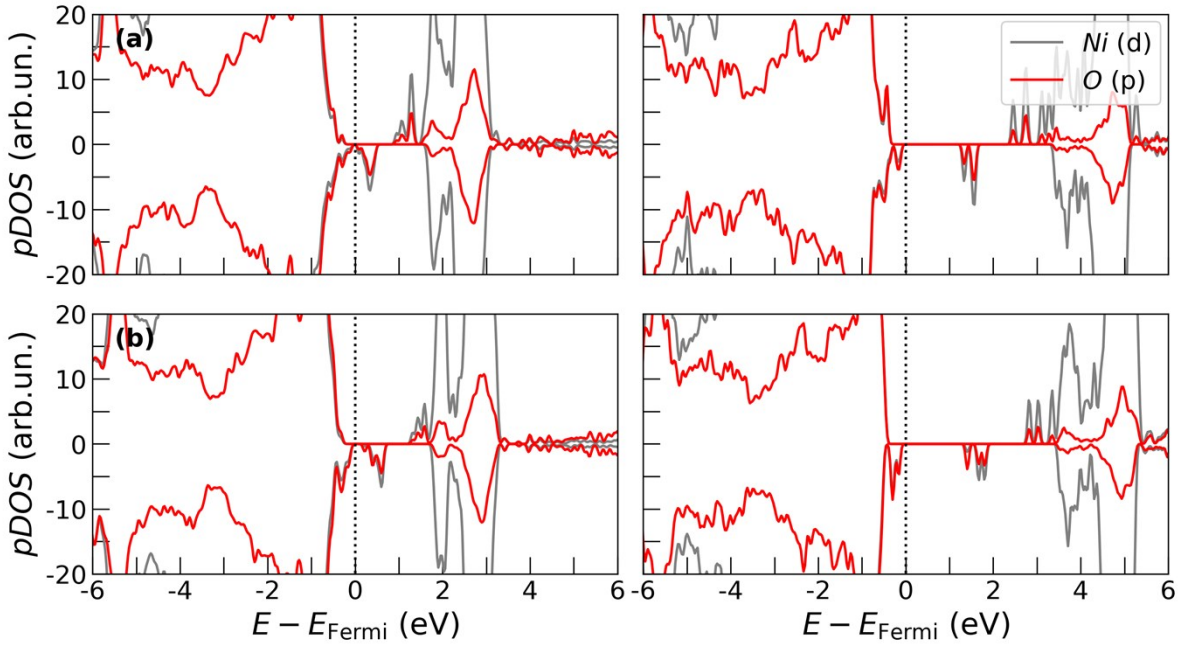

Figure S2. Spin-resolved atom-angular momentum-projected densities of states (pDOS) at PBE+U (left side) and HSE (right side) theory level calculated for the doped surface slab models: NiO:VNi:Li (panel a), NiO:VNi:Ag (panel b).

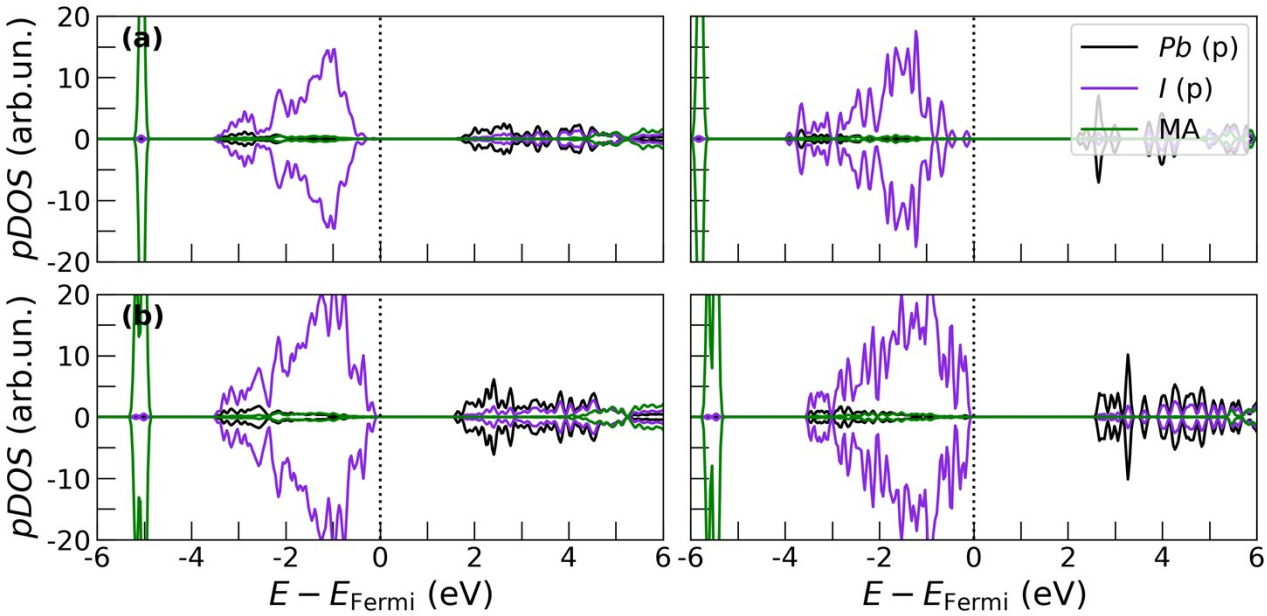

Figure S3. Spin-resolved atom-angular momentum-projected densities of states (pDOS) at PBE+U (left side) and HSE (right side) theory level calculated for the MAPI bulk (panel a) and for the PbI_2-terminated slab surface (panel b).

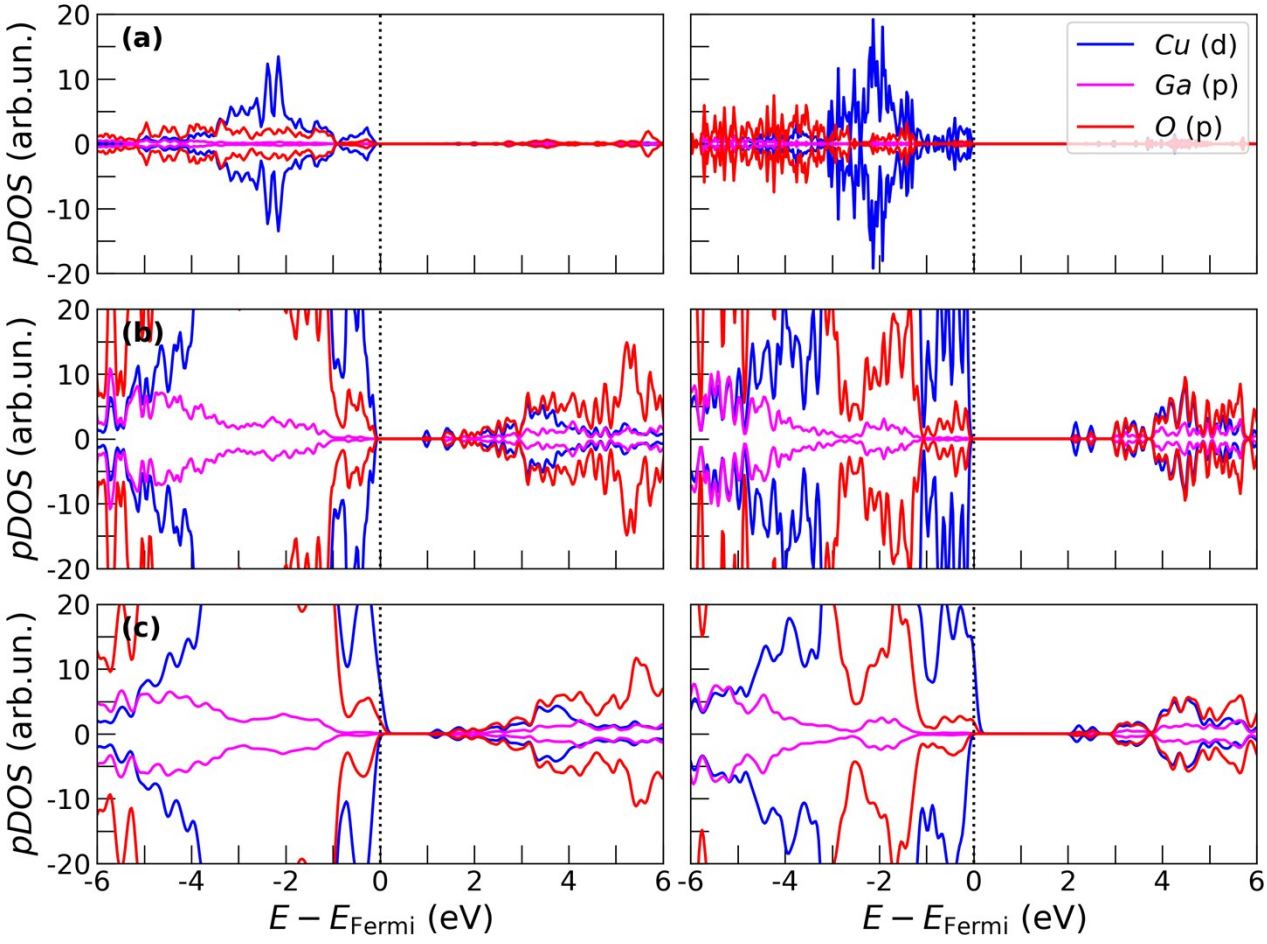

Figure S4. Spin-resolved atom-angular momentum-projected densities of states (pDOS) at PBE+U (left side) and HSE (right side) theory level calculated for the

$CuGaO_2$ bulk (panel a), for pristine slab surface (panel b) and for the $CuGaO_2$:V_{Cu} slab surface model.

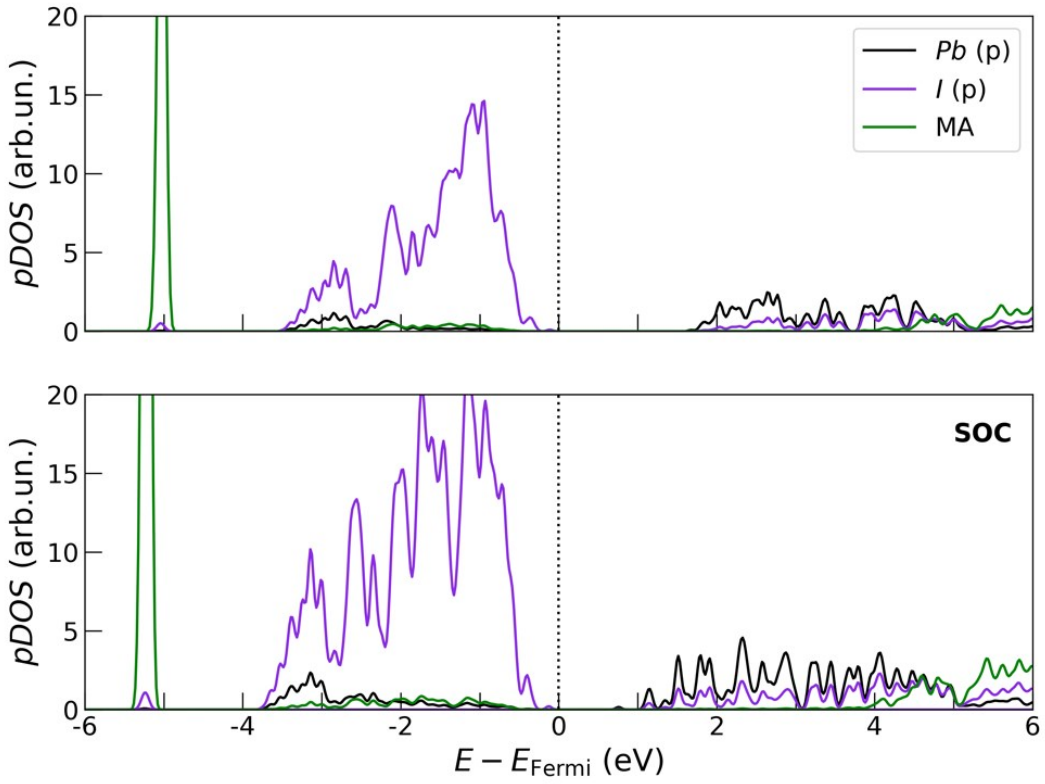

Figure S5. Atom and orbital momentum-projected density of states (pDOS) of the MAPI slab without (upper panel) and with (lower panel) spin-orbit coupling (SOC) contribution, calculated at PBE theory level.

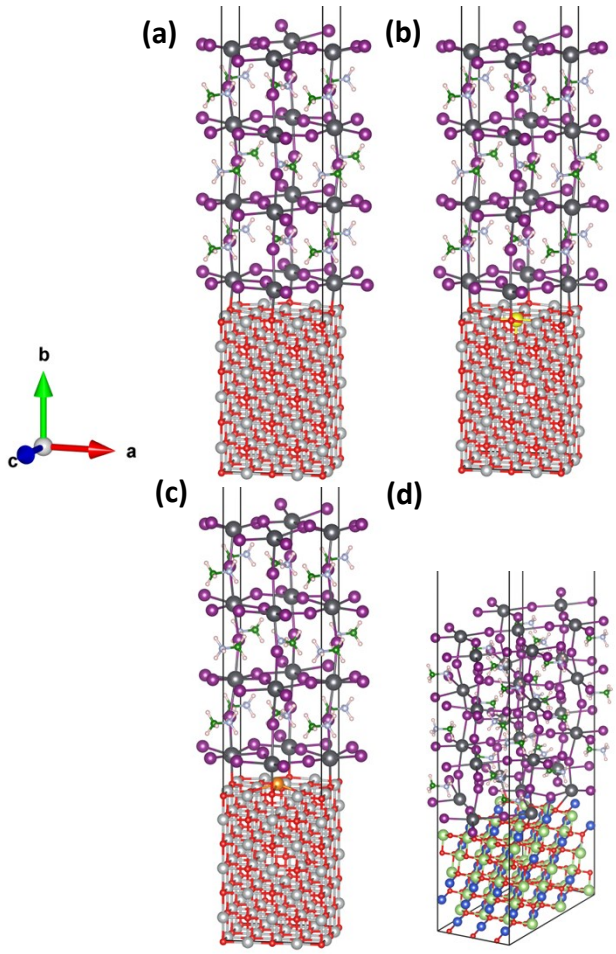

Figure S6. Minimum-energy structures of MAPI/HTL interfaces with (a) NiO (a), (b) NiO:V_{Ni}:Li (b), NiO:V_{Ni}:Ag (c) and $CuGaO_2$ (d). Color legend as in Figure 1 of the paper.

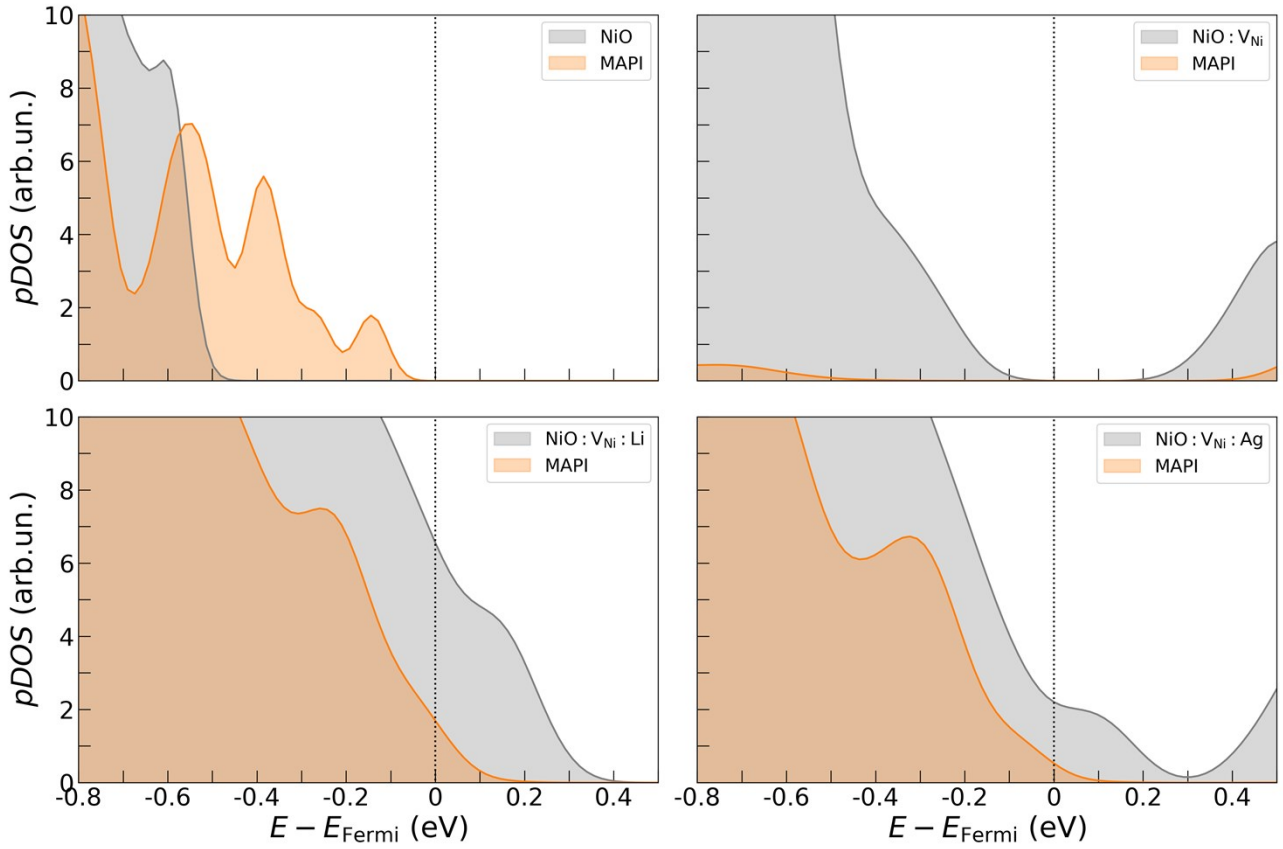

Figure S7. Magnification around the Fermi energy of the projected density of states (PDOS) plots for MAPI/NiO heterojunctions, computed at the PBE+U level.

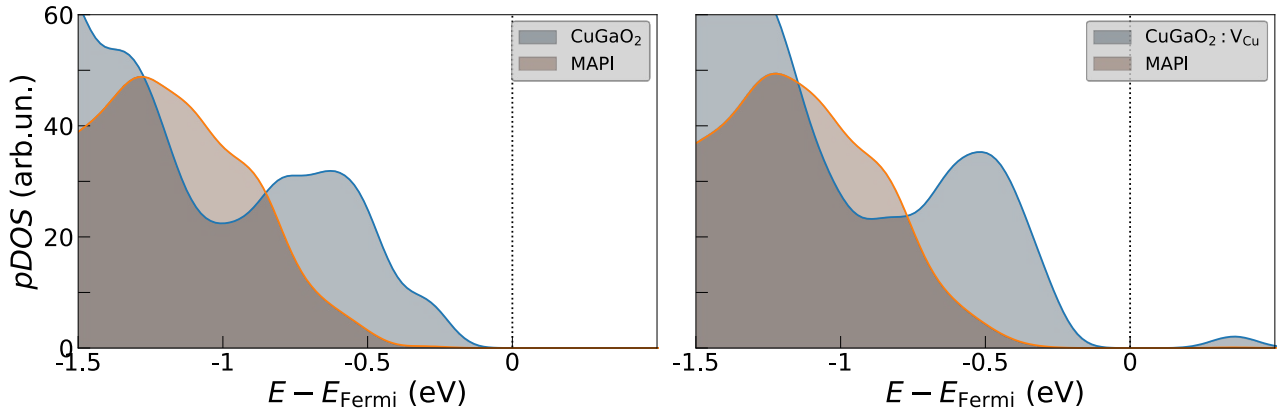

Figure S8. Magnification around the Fermi energy of the projected density of states (PDOS) plots for MAPI/$CuGaO_2$ heterojunctions, computed at the PBE+U level.

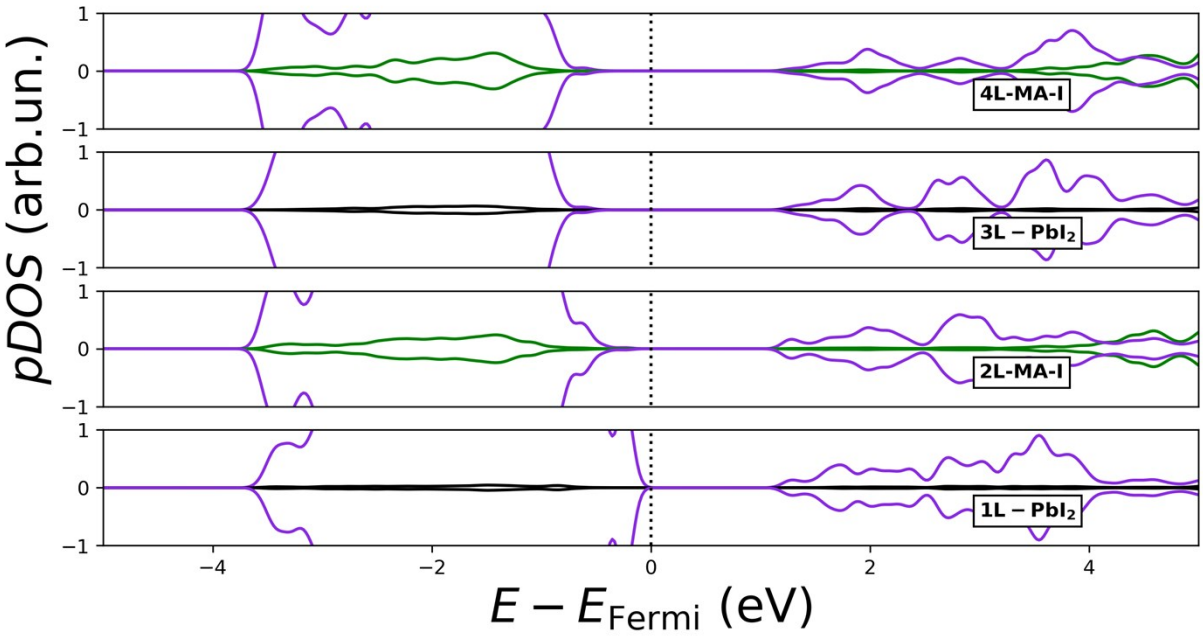

Figure S9. Layer-resolved PDOS plots computed at the PBE level of theory on MAPI isolated slab at the geometry of MAPI/$CuGaO_2$:V_{Cu} heterostructure.