

PHYSICAL PROPERTIES OF INTERFACES BETWEEN TiO₂ AND PEROVSKITES WITH QUASIPARTICLE DFT-1/2 CORRECTION

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INTRODUCTION AND GOAL

- Interfaces between layers play a crucial role for efficiency of the solar cell.
- We aim to study theoretically interfacial properties by means of the explicit heterostructure using DFT-1/2 [1, 2].

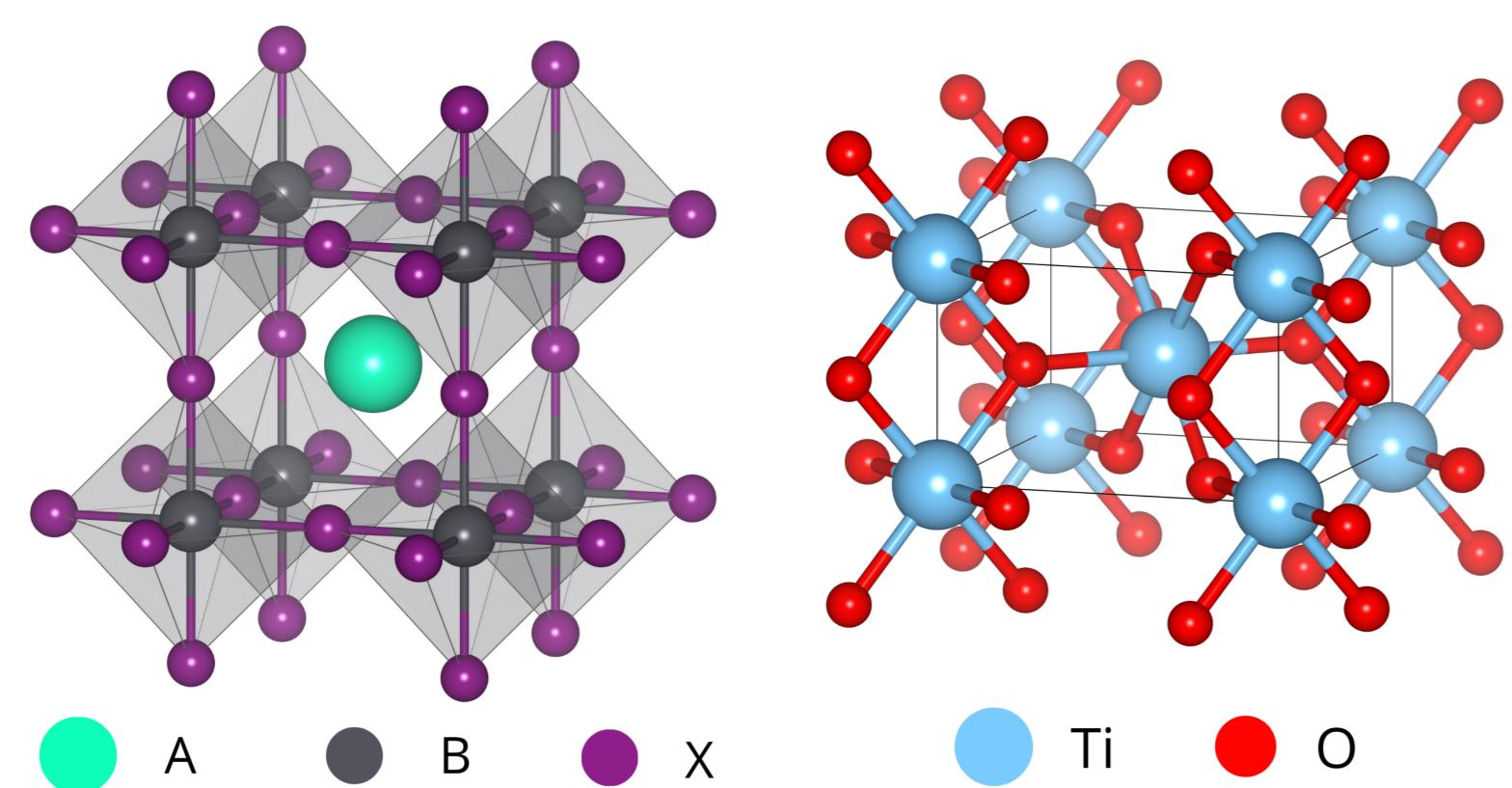


Figure 1: Perovskite (ABX₃) and TiO₂ nanostructures

METHODOLOGY

- All calculations run on VASP code [3].
- Removal of half electron from the most predominant orbital in the valence band for DFT-1/2 implementation using the software minushalf [4].
- Heterostructure with 22 atomic layers and 405 atoms in total.
- Projected density of states in each atomic layer.

CONCLUSIONS

- The quasiparticle correction DFT-1/2 and SOC implementation provided accurate values for the compounds properties.
- This method provides a rigorous description of real interfaces, going beyond the simplified models presented in the literature.
- With quasiparticle correction, the band alignment tends to approximate from type 2, but it is required SOC effect employment for further description.
- It is necessary a longer heterostructure to achieve bulk properties.

RESULTS AND DISCUSSIONS

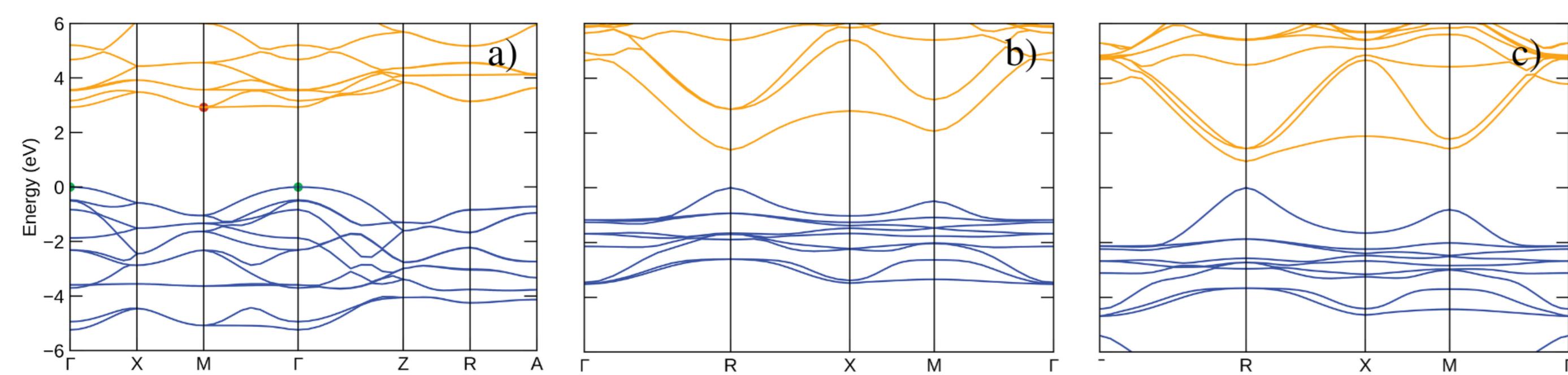


Figure 2: Band structure of (a) TiO₂, (b) CsPbI₃ and (c) CsSnI₃

Compound	lattice parameter (Å)			bandgap (eV)						
	a	c	(s)a	(s)c	DFT	DFT-1/2	SOC + DFT-1/2	Exptl	(s)	SOC + DFT-1/2
TiO ₂	4.670	2.967	-	-	1.717	2.924	2.924	3.051 [5]	-	-
CsPbI ₃	6.388	6.388	7.005	6.242	1.472	2.545	1.385	1.68 [6]	1.612	-
CsSnI ₃	6.270	6.270	7.005	6.108	0.450	1.348	0.967	1.27 [7]	1.523	-

Table 1: Lattice parameter (Å) and bandgap (eV) of the bulk and bulk strained (s) for cubic and tetragonal structures

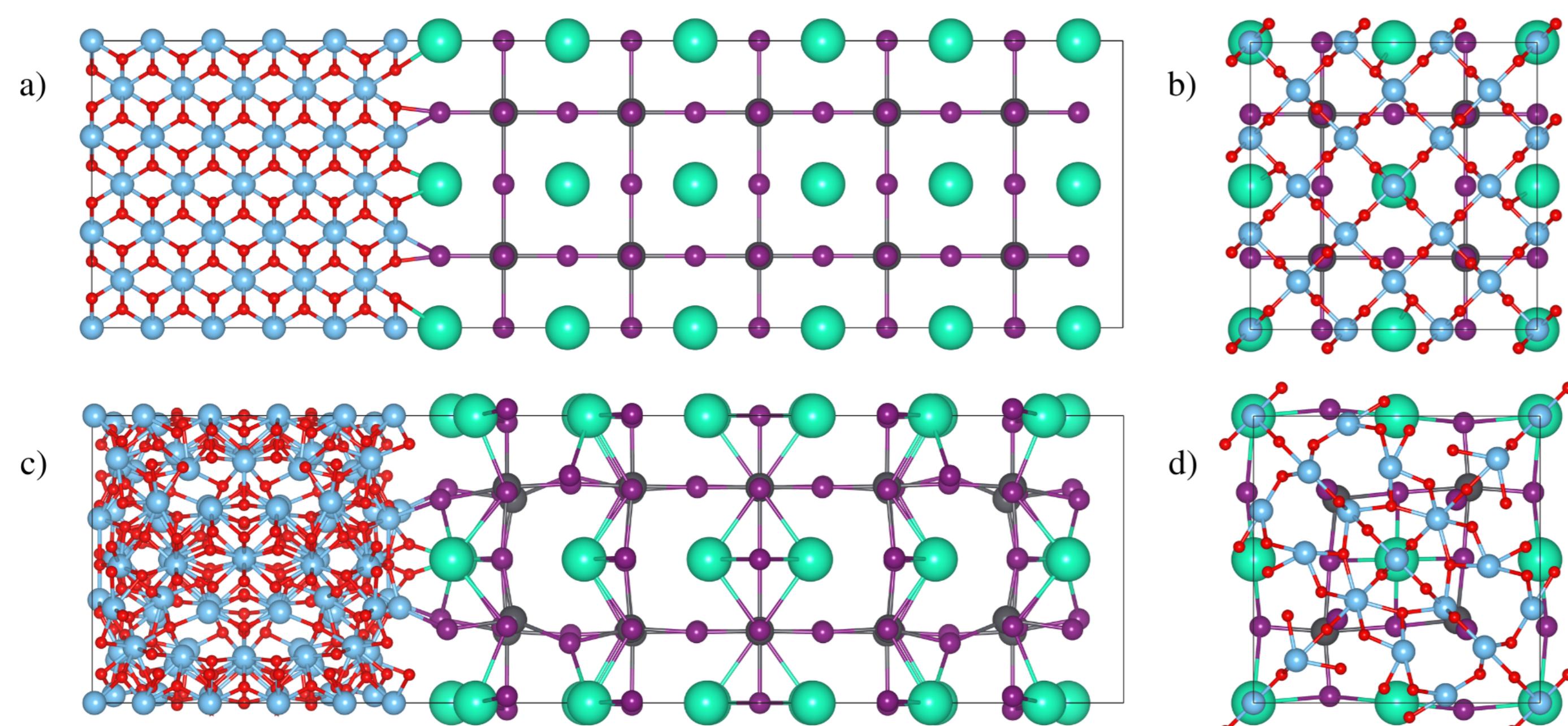


Figure 3: Heterostructure (a) non-relaxed, (b) the 4 layers of contact, (c) relaxed and (d) its 4 layers of contact

VBO	CBO	bandgap (TiO ₂)	aim	bandgap (CsPbI ₃)	aim
DFT	2.617	1.771	1.914	1.717	1.213
DFT-1/2	4.306	3.101	3.617	2.924	2.412

Table 2: Valence (VBO) and conduction (CBO) band offset and bandgap in the middle of each side, all in eV

- Previously works provide average values of 2.285 eV and 0.637 eV for VBO and CBO [8-10], all values with respect to the vacuum level. However, there is a lack of works that calculate the energy alignment for the heterostructure. This is what we desire obtain.

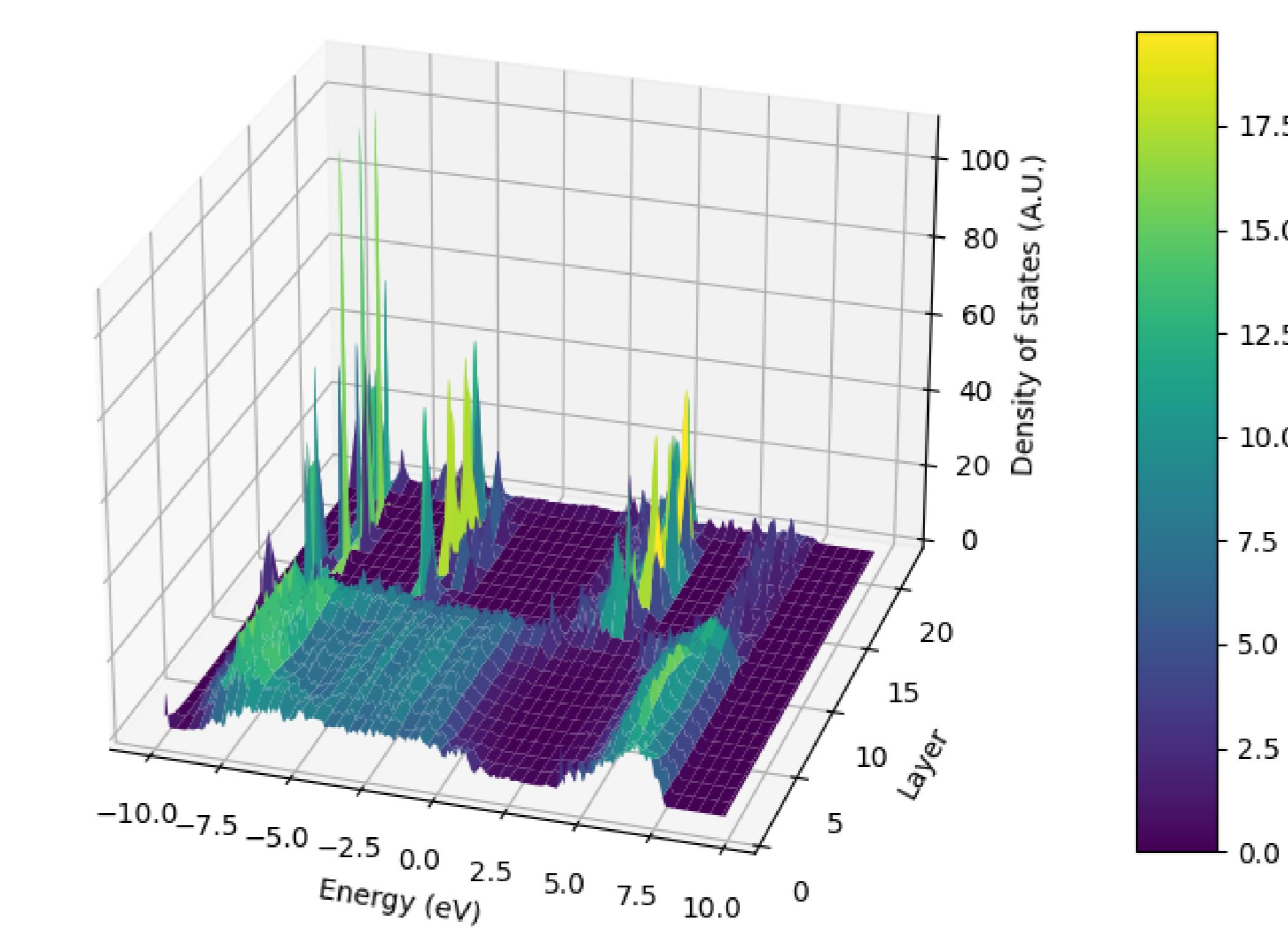


Figure 4: Projected density of states in each layer

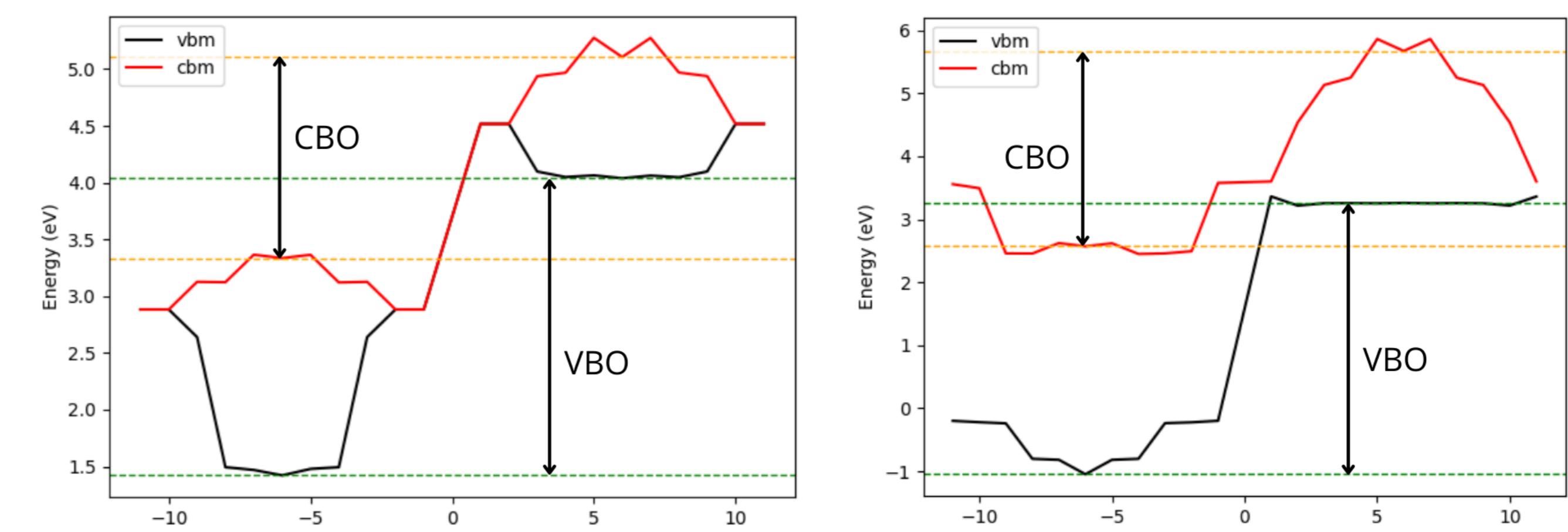


Figure 5: Band alignment for TiO₂ - CsPbI₃ heterostructure using DFT (left) and DFT-1/2 (right)

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