

Photoelectron extraction in BiOI: an atomistic perspective

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S1: Charge density difference (CDD) maps

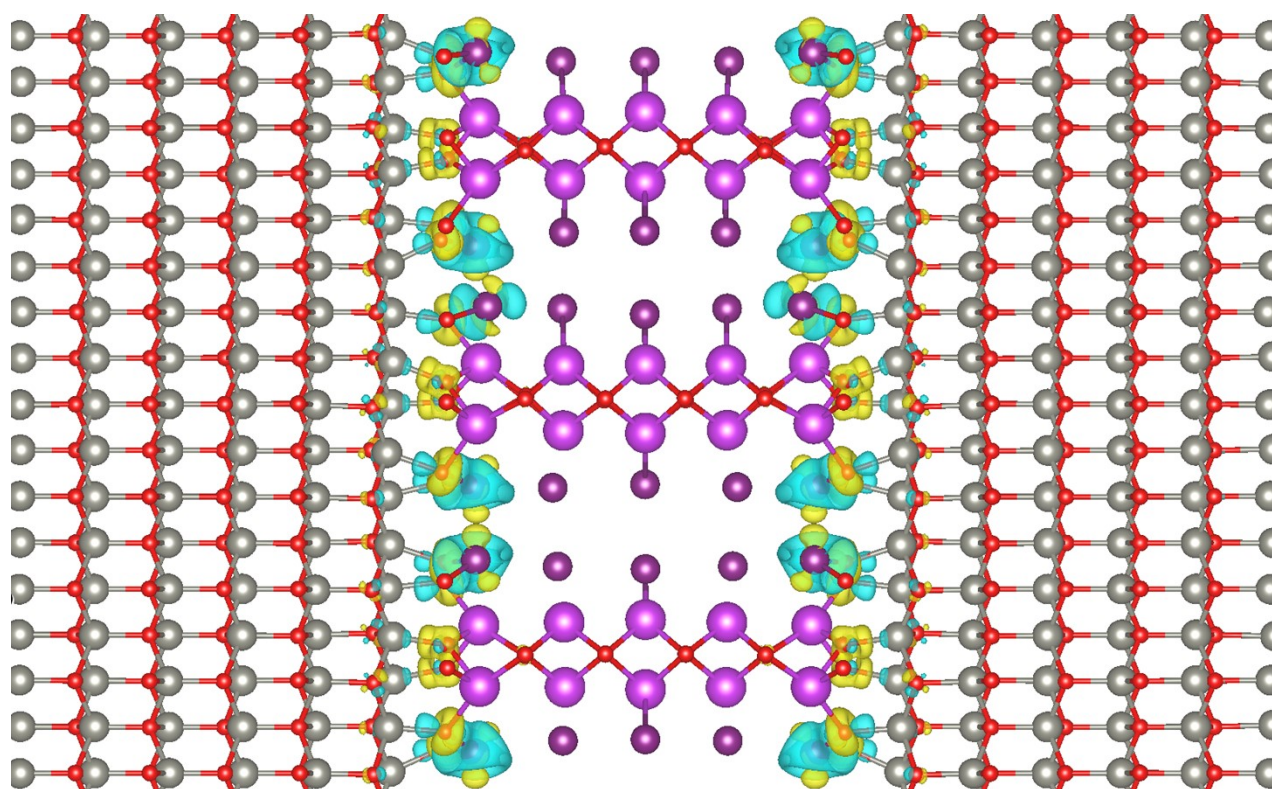


Figure S1: Charge density difference between the composite structure and BiOI and both the ZnO structures computed as $\Delta\rho(x) = \rho_{\text{ZnO}^1/\text{Bi}/\text{ZnO}^2}(x) - (\rho_{\text{ZnO}^1} + \rho_{\text{Bi}} + \rho_{\text{ZnO}^2})$. Here, yellow lobes correspond to charge accumulation, whereas cyan lobes indicate charge depletion.

Table S1: Average Bader Charge

I in bulk BiOI	I at the BiOI/ZnO interface	O in bulk ZnO	O bonded with I atoms at the BiOI/ZnO interface
-0.51 e	1.93 e	-1.22 e	-1.65 e

S2: pDOS of BiOI/defected ZnO heterojunction.

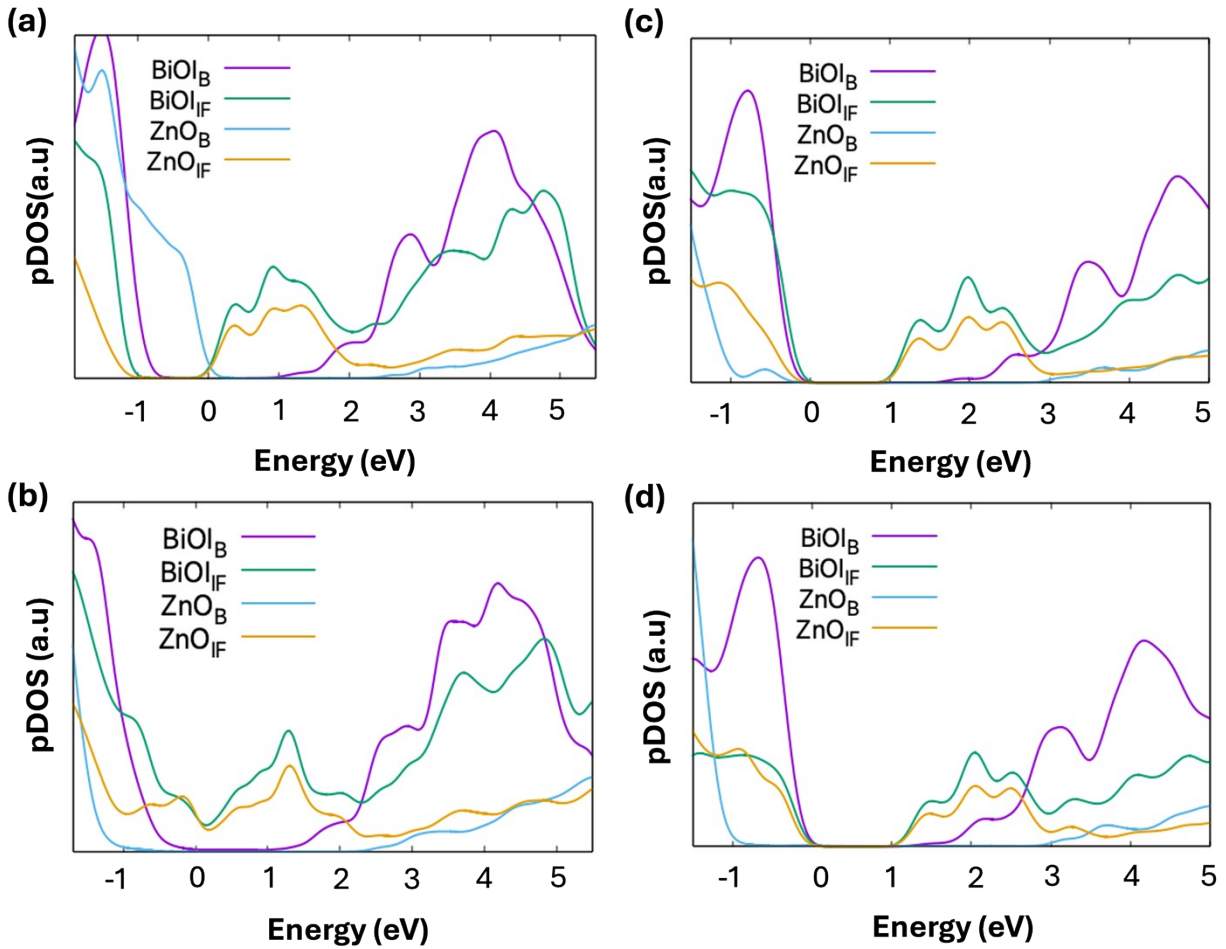


Figure S2. Density of states projected on the bulk (B) and interface (IF) layers of BiOI and defected ZnO: a) V_{Zn}'' in the bulk; b) V_{Zn}'' at the interface; c) O_i'' in the bulk; d) O_i'' at the interface.