Supplementary Material for Physical insight of Random Fluctuation in Metal/IGZO Schottky Barriers for Low-Variation Contact Optimal Design

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As you mentioned, cutoff energy can affect the reliability of the results. Therefore, we have recalculated the data using the correct cutoff energy and have also conducted convergence testing.
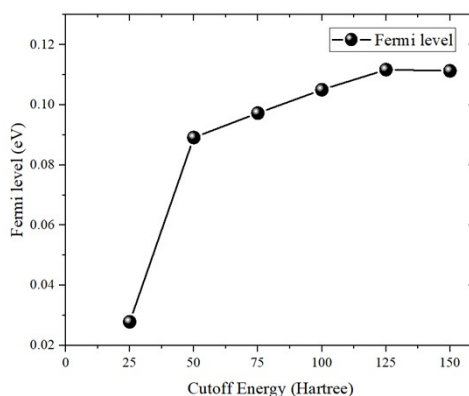

Fig. S1 The results indicate the relationship between the cutoff energy and Fermi level.

It was observed that the convergence was achieved when the cutoff energy exceeded 50 Hartree. By using a cutoff energy of 125 Hartree, we could further the improve the computational accuracy. Therefore, a cutoff energy of 125 Hartree was selected for the subsequent calculations.

Table S1: Binding energy (E_b) of different metals with Surface: A

	Au	Al	Mo	Ti
E_b (meV/Å²)	-62.01	-74.80	-100.93	-185.66

For the majority of van der Waals contacts, $|E_b|$ is around 20 meV/Å². (DOI: 10.1103/PhysRevLett.108.235502). Our system is significantly greater than this value, therefore our contact type is binding contract.
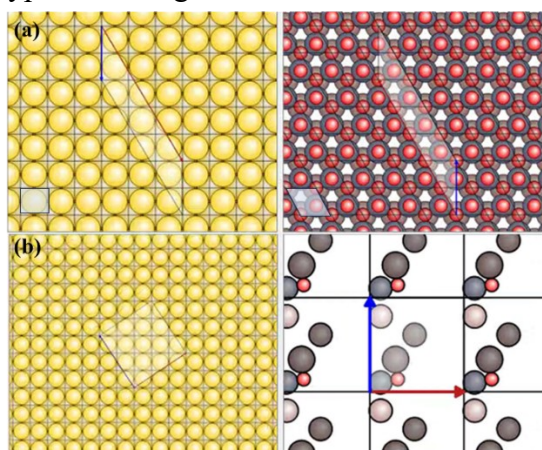

Fig. S2 Cross-sectional schematic of the heterojunction interface, with (a) and (b)

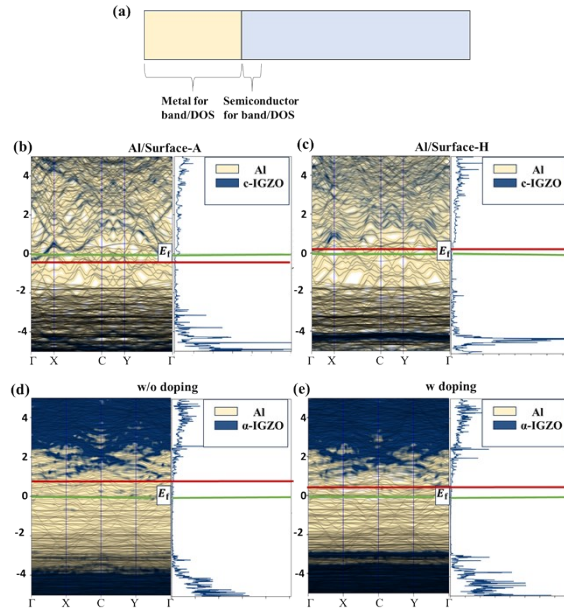depicting a schematic diagram of c-IGZO and a-IGZO, respectively.

Fig. S3： (a) The projected band structure and density of states （DOS）for a heterojunction system. Metal site is fully projected onto the band structure, while the semiconductor part is only projected near the interface. (b) and (c) show the projected band structure and DOS of metal Al and the interface surface-A/H. (d) and (e) display the projected band structure and DOS of amorphous IGZO(α-IGZO) before and after interface doping. The red solid line represents the Conduction band minimum (CBM), and the green solid line represents the Fermi level (E_f).

We observed that in Fig. S3 (b), the CBM of c-IGZO is lower than the E_f, indicating Ohmic contact. Conversely, in Fig. S3 (c), Schottky contact is observed. Furthermore, from the analysis of Fig. S3 (d) and (e), it is found that interface doping leads to a reduction in the position of the CBM, resulting in a decrease in the Schottky barrier height.