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Properties of Homo- and Hetero- Schottky Junctions from First Principle Calculations

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Supporting Material:

Energy resolved local density of states (LDoS) of *n*-type doped Si thin film with doping concentration of 10^{19} cm^{-3} is shown in Fig. S1. The energies reference is taken to be the chemical potential of metal and Si at zero bias across the Schottky barrier. In contrast to the intrinsic Si film (see Fig. 2 in the main text), the band bending is upward at the interface. Doping of the Si thin film has been implemented using "compensation" charge concept that has been introduced in the localised basis sets [S1,S2].

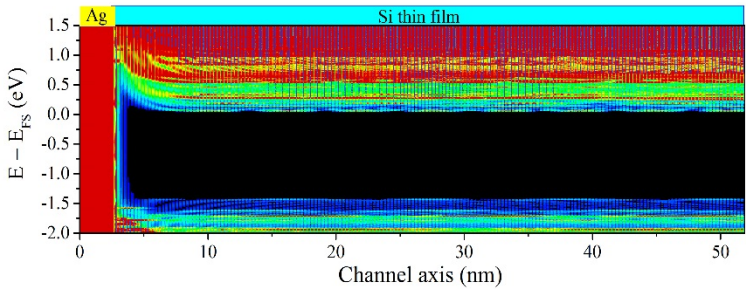


Fig. S1. Equilibrium energy resolved local density of states (LDoS) of Ag/Si interface. The Si thin film is *n*-type doped with the doping concentration of 10^{19} cm^{-3}.

The difference between the charge difference density (CDD) at +1 V and equilibrium, and at −1 V and equilibrium is extracted for the thick/thin α-Sn structure and the cut-planes in the centre of cross-section along the channel are shown in Figs. S2(a) and S2(b). Blue and red correspond to charge depletion and charge accumulation, respectively. Similarly, the difference between the CDD of Ag/intrinsic Si Schottky barrier under +1 V / −1 V and equilibrium is shown in Figs. S2(c) and S2(d). Due to smaller band gap of the thin (semiconducting) α-Sn film the external gate bias modifies the bands (see Fig. 3(a) in the main text) such that DoS exists at the Fermi energy at both +1 V and −1 V biases, hence, creating gate-induced ambipolar behaviour as can be seen in Figs. S2(a) and S2(b). This behaviour, however, is not as pronounced in the Ag/Si structure due to larger Si thin film band gap.

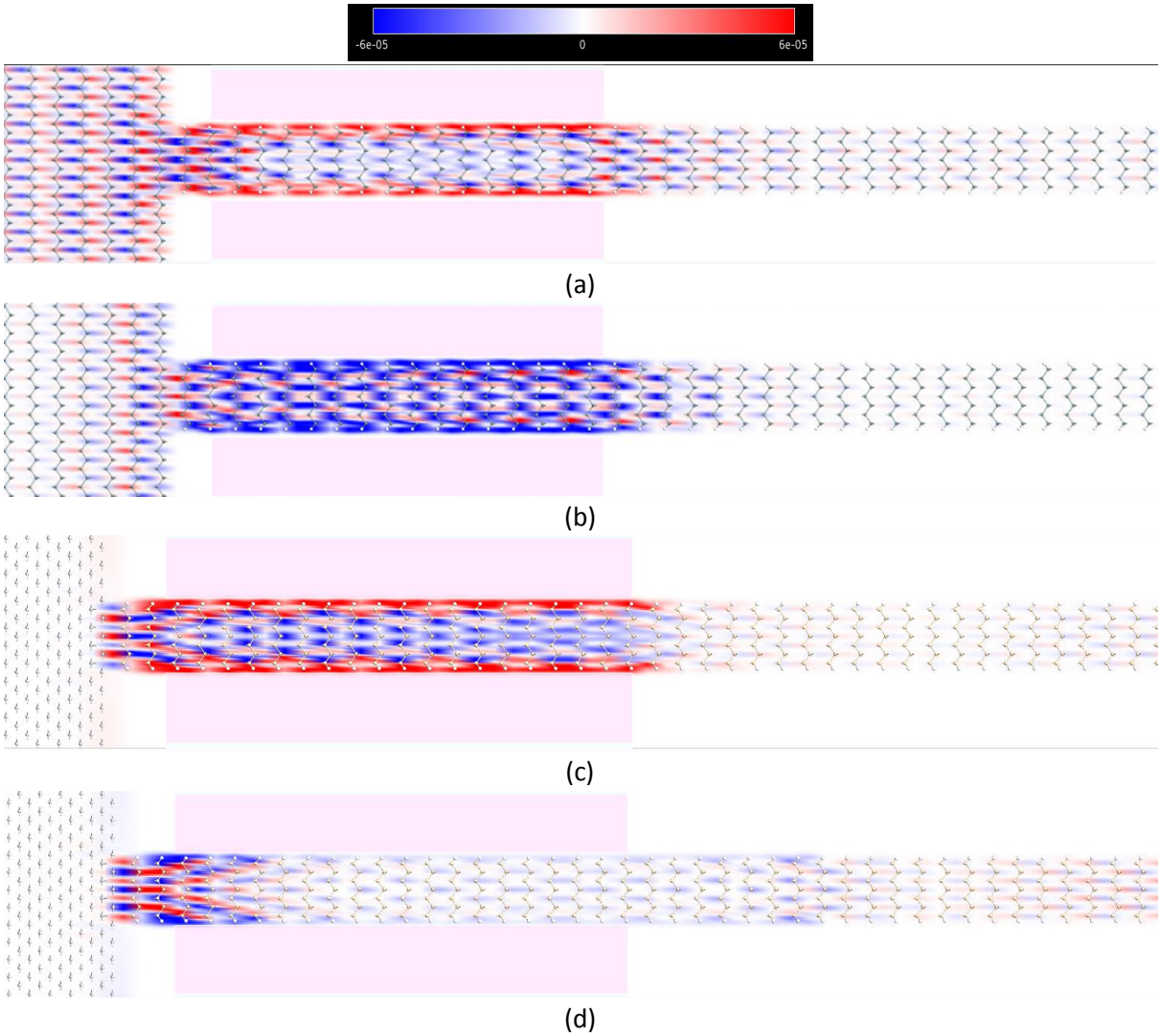


Fig. S2. The difference between CDD for thick/thin monomaterial junction at (a) +1 V and equilibrium, and (b) −1 V and equilibrium, and for Ag/Si junction at (c) +1 V and equilibrium, and (d) −1 V and equilibrium.

References

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