Electronic Supplementary Material (ESI) for Faraday Discussions.

Supplementary Information for

Structural transition pathway and bipolar switching of the GeTe–Sb_2Te_3 superlattice as interfacial phase-change memory

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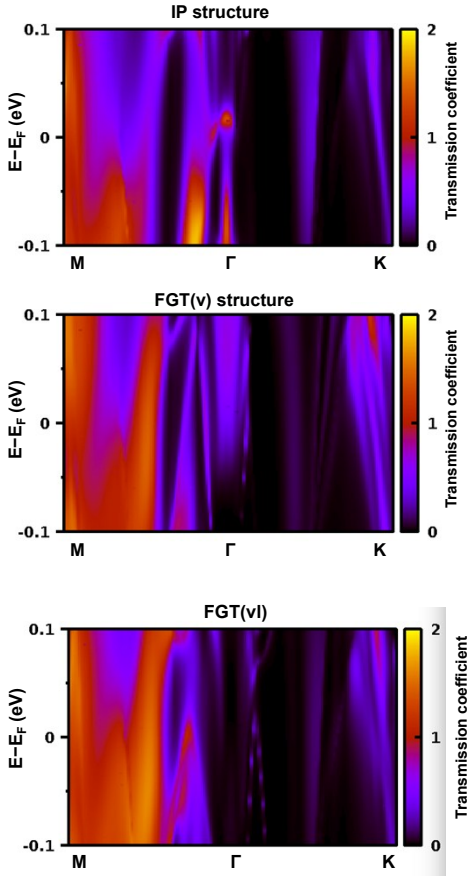
SI. 1. Contour plots of the transmission coefficient

In the Figure SI. 1, we show the calculated transmission coefficients as a function of the energy E and the wave vector $\vec{k}_{//}$. The transmission coefficient resolved by $\vec{k}_{//}$ can be calculated as follows:

$$T(E,\vec{k}_{//}) = \mathrm{Tr}[\Gamma_R(E,\vec{k}_{//})G(E,\vec{k}_{//})\Gamma_R(E,\vec{k}_{//})G^{\dagger}(E,\vec{k}_{//})]$$

where G is the (retarded) Green's function by the Bloch Hamiltonian $H(\vec{k}_{//})$ and $\Gamma_{L/R}$ is $i(\Sigma_{L/R} - \Sigma_{L/R}^{\dagger})$ where $\Sigma_{L/R}$ is the self-energy of the left/right leads. The upper, middle and lower panels are the contour plots of the transmission coefficient of IP, FGT(v), and FGT(vl) structures, respectively.



SI. 2. Voltage drop profiles

In the Figure SI. 2, we show the voltage drop in the adopted device model when the applied bias is 1.5 Volt. The profiles of voltage drop is defines as V_H(z,V=1.5 Volt)−V_H(z,V=0.0 Volt), where V_H is the self-consistent Hartree potential obtained by NEGF-DFT, and z is the coordinate along the transport direction (c-axis). The upper panels are the plots of IP (left), TS(V1) (middle) and FGT(v) (right), respectively. The lower panel is the schematic view of the calculated device cell to identify atomic positions.