Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information for

Resistive switching mechanism of GeTe-Sb_2Te_3 interfacial phase change memory and topological properties of embedded two-dimensional states

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<u>SI. 1.</u> **Structure parameters of the unit cell of GST-SL [$(QL)_2(GeTe)_2$]**

Structure	*a* (*b*)	*c*	ΔE_{tot}
IP	4.23	27.8	0.00
P(v)	4.19	29.2	0.42
P(vl)	4.24	27.4	-0.11
FGT(v)	4.22	28.1	0.26
FGT(vl)	4.25	27.3	-0.17

Table SI. 1. Structure parameters of [$(QL)_2(GeTe)_2$] unit of GST-SL by fully relaxation of atomic positions and lattice constants. (in Ang unit). The lattice constants of *a*,*b* and *c* axis are listed. The energy ΔE_{tot} is the energy difference of the unit cell from the energy of IP structure. The unit is eV.

<u>SI. 2.</u> Bond lengths of the atoms (IP structure) in the $[2,2]_{ref}$ and $[2,2]_{elng}$ units.

$[(2,2)_{ref}]$

Te^2-Te^3	Te^2-Te^2	Sb-Te^1	Sb-Te^2	Ge-Te^3	Ge-Ge
3.86	3.79	3.16	3.00	2.81	2.95

$[(2,2)_{elng}]$

Te^2-Te^3	Te^2-Te^2	Sb-Te^1	Sb-Te^2	Ge-Te^3	Ge-Ge
4.18	3.71	3.16	2.99	2.81	2.95

Table SI. 2. Bond length of IP structure $[(2,2)]_{ref}$ and $[(2,2)]_{elng}$ of GST-SL used for the RSLs. The unit is Ang. The index number for each atom is given in Figure 1(b) while Te^2-Te^2 is distance of the nearest neighboring Te atoms in the neighboring QL layers by staking [(2,2)] periodically along c-axis direction.

<u>SI. 3</u>. Contour plots of the interface states of QL/GeTe in the RSL of iPCM device.

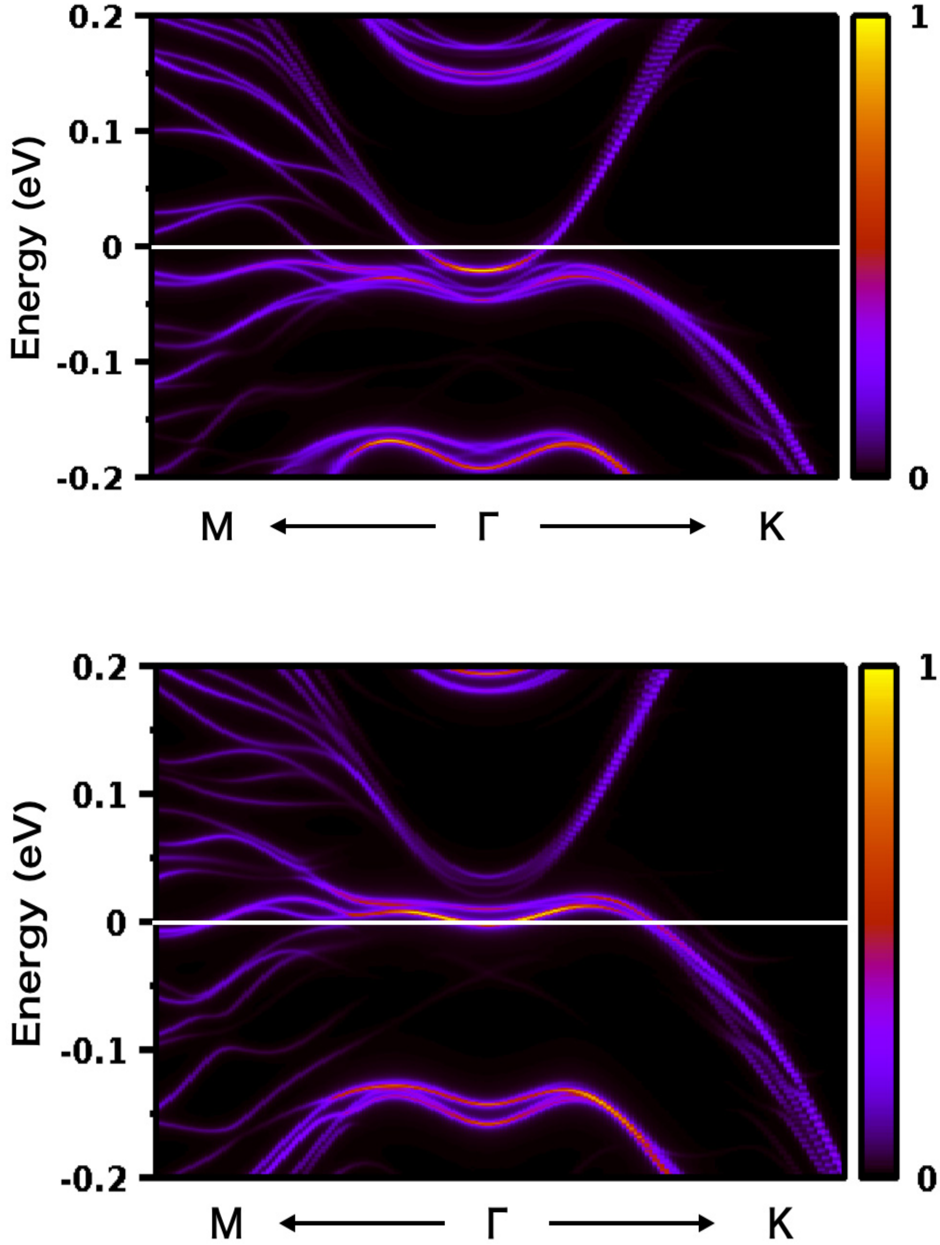

Figure SI. 1

The contour plots of the density of states of the surface states and interface states for the inverted Petrov phase as a function of electron energy E and the wave vector $\vec{k}_{//}$ (2D band dispersion). QL/GeTe interface states in the iPCM device of $W/[(2,2)_{ref}]_3/(QL)_2/W$ for V= 0 Volt (upper panel) and V=0.5 Volt (lower pannle), respectively. The zero of energy is set to E_F of of electrode (W bulk). The unit of density of states is arbitrary.

<u>SI. 4.</u> Contour plots of the transmission coefficient

In the Figure SI.2, we show the calculated transmission coefficients as a function of the energy E and the wave vector $\vec{k}_{//}$ for the device model $W/[(2,2)_{ref}]_3(QL)_2/W$. 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 the lower panels are the contour plots of $\log_{10} T(E,\vec{k}_{//})$ for IP, P(v), and FGT(vl) structures, respectively. For each structure, the plots are the result by V=0 Volt (left panel) and 0.5 Volt (right panel), respectively.

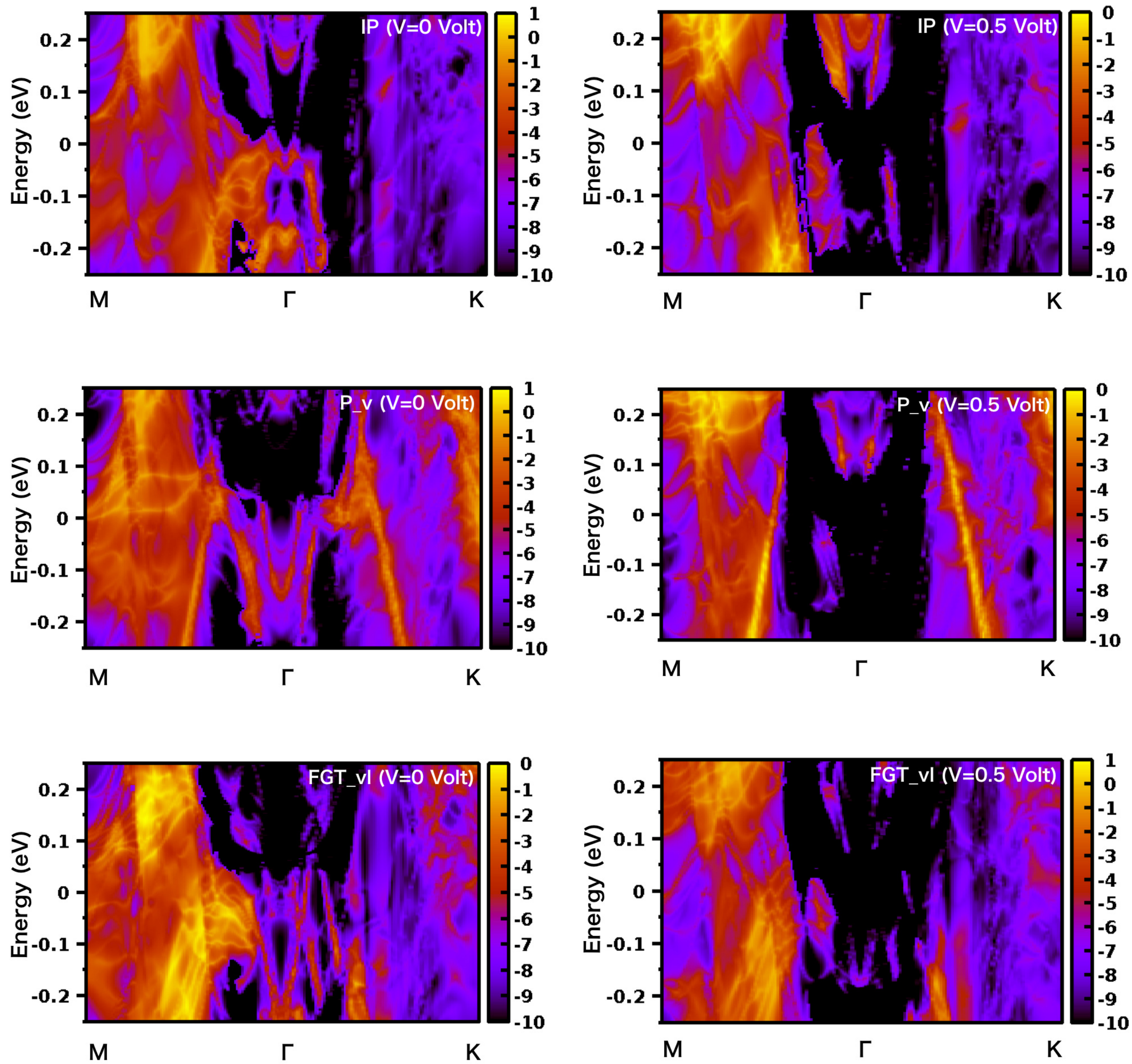

Figure SI. 2

The upper, middle and the lower panels are the contour plots of $\log_{10} T(E,\vec{k}_{//})$ for IP, P(v), and FGT(vl) structures, respectively. For each structure, the plots are the result when the applied bias V is 0 Volt (left panel) and 0.5 Volt (right panel), respectively.