Electronic Supplementary Information

Silicon compatible Sn-based resistive switching memory

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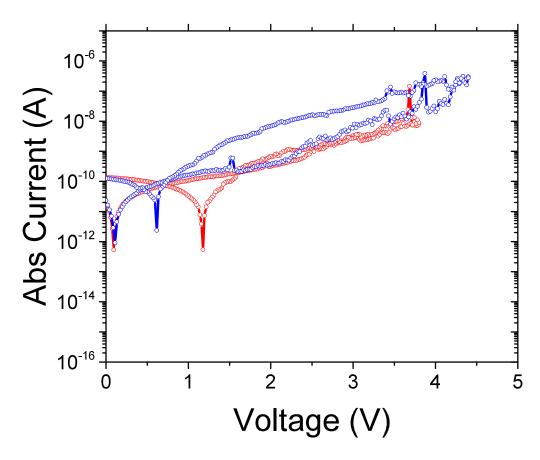


Figure S1. Current-Voltage characteristics measured on Sn|HfO₂|Pt device in pristine condition with Pt as the anode (positive bias applied to Pt). No resistive switching is seen for comparative voltage bias range.

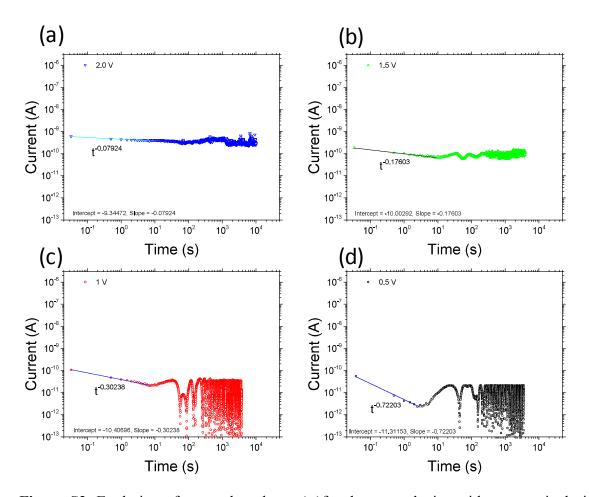


Figure S2. Evolution of power law decay (t^n)for the same device with progressively increased voltage stress: (a) V=2.0 V, n=-0.079, (b) V=1.5 V, n=-0.176, (c) V=1.0 V, n=-0.302, (d) V=0.5 V, n=-0.722.

Atomistic diffusion pathway for Sn in HfO₂:

The fundamental diffusion pathways of Sn in HfO₂ are still poorly understood. Density functional theory (DFT) calculations were first performed to identify the most energetically favorable configuration of Sn in HfO₂. Sn can possibly exist in interstitial, substitutional sites in pristine HfO₂. Amongst all these possible configurations, our DFT calculations suggest that the interstitial site *i.e.* the octahedral site in which a Sn atom is surrounded by six Hf atoms, is favored energetically. Nudged Elastic Band Calculations (NEB) calculations were therefore performed to compute the barrier for Sn diffusion from one octahedral interstitial. In the initial state, the Sn atom is surrounded by four oxygen atoms. When the Sn atom moves to the transition state with the highest distorted site, it is repelled by its two nearest neighboring O atoms from both sides, leading to an energy increase of 0.54 eV. After the transition state, the distance between Sn and its nearest neighboring O atoms increases to release the stress, so that the total energy reduces. At the final state with Sn occupying the adjacent octahedral site, its geometrical structure is identical with the initial state.