Theoretical studies of metal | transition metal dichalcogenides | metal vertical stacks: atomristors

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Since the discovery of graphene and technologies to fabricate it, the share of 2D materials in nanotechnologies has consequently increased in the past few years [1,2]. In the 2D material family, transition metal dichalcogenides (TMDs) exhibit a resistive switching behaviour [3-5] in metal|TMD|metal vertical stacks, which would allow a switching time for radio-frequency switches of less than 10fs [6], when nowadays switches have a value ten times greater [7]. While the migration of metallic ions forming filaments in metal|hBN|metal systems has been found to be the main source of switching [8], no such claim has yet been made using TMDs. A recent theoretical study [4] using Au electrodes has shown that the creation of a half-filament is enough to trigger the low-resistance state (LRS), while a full filament would require a vast amount of energy to form. The presence of defects affects little the high-resistance state (HRS), but does provide a higher probability of creating a half-filament.
Using density-functional theory and non-equilibrium Green's functions, this work concentrates on understanding the mechanisms of this switching in TMD systems, changing the electrode materials as well as the nature and phase of the TMDs in question. A database of devices with possible electrodes made of Au, Ag, Cu, Ni, Pt and TiN and mono-, bi-, tri-layered TMDs $\{Mo;W\}\{S;Se;Te\}_2$ is being built in order to establish a precise comparison of the HRSs and LRSs. Additional systems including hBN and graphene have also been investigated as possible footstones.

References

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