Resistive switching in memristors based on 2D materials

Zineb Kerrami[1], Gaelle Bigeard[1], François Triozon[2], Alessandro Cresti[1]
[1] *Univ. Grenoble Alpes, Univ. Savoie Mont Blanc, CNRS, Grenoble INP, CROMA, 38000 Grenoble, France*
[2] *CEA-Leti, 17 avenue des Martyrs, 38054 Grenoble, France*
zineb.kerrami@grenoble-inp.fr

The resistive switching mechanism in atomristors is driven by an external electric field that induces the migration of metallic ions from the contacts to the 2D material. The resulting conductive filament connects the electrodes, enabling different resistance states [1]. However, understanding the physics behind filament evolution and device performance remains a complex challenge. In this study, we employ density functional theory and non-equilibrium Green's function method to investigate the electronic and transport properties of monolayer and multilayer 2D materials sandwiched between two metallic electrodes. We consider structural defects and substitutional doping as key factors in the transition from low resistance state (LRS) to high resistance state (HRS). Our examination includes various 2D materials such as 1T-MoS_2 and 2H-MoS_2 (representing conductor and semiconductor phases of TMDs), graphene, and hBN. We illustrate how the electrical conductivity could be influenced by the thickness of the 2D material and the electronic behaviour at the interface with the electrodes. Furthermore, we investigate the effect of atomic vacancies and metal ion substitutions on the transport properties. These defects introduce localized states within the bandgap, which alter the electronic properties and then affect charge transport across the 2D material, thus enabling resistance switching between LRS and HRS.

References

[1] R. Ge *et al.*, Nano Lett., 18 (2018) 434.

Figures

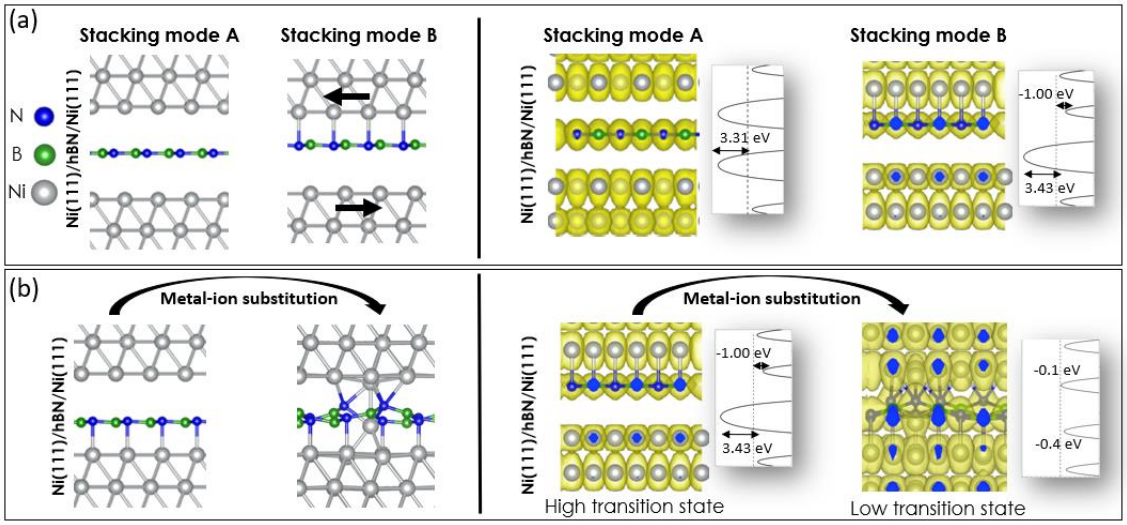

Figure 1: (a) Structural illustration (Left) and charge distribution (Right) of hBN in different stacking modes. Inset figure shows the averaged electrostatic potential. Reduced tunnelling barrier due to N-Ni bond formation at the interface in stacking mode B. (b) Structural illustration (Left) and charge density distribution (Right) of pristine and defected Ni/hBN/Ni systems. Charge distribution reveals enhanced charge density at the interface, attributed to the effect of metal-ion substitution. The averaged electrostatic potential shows no tunnelling barrier after metal-ion substitution, which indicates higher electronic transmission and then higher conductivity.

Acknowledgements

This work is supported by the LabEx Minos under the contract ANR-10-LABX-55-0, and by the ANR SWIT Grant (ANR-19-CE24-0004). It is implemented using HPC resources from GENCI–IDRIS (Grant 2023 A0140914157), GENCI–TGCC (Grant 2024 AD010914993), and the GRICAD infrastructure (https://gricad.univgrenoble-alpes.fr), which is supported by Grenoble research communities.