Resistive switching in atomristors: Insights from DFT and NEGF study

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The resistive switching mechanism in atomristors plausibly lies in an external electric field-driven migration of metallic ions from the contacts to the 2D material. The resulting conductive filament connects the electrodes, thus enabling different resistance states [1]. The physics behind the filament evolution and the device performances remains a complex issue to be addressed. In this study, we employ density functional theory (DFT) and non-equilibrium Green's function (NEGF) method to investigate the electronic and transport properties of monolayer and multilayer 2D materials sandwiched between two metallic electrodes. Structural defects and substitutional doping have been considered as activators for resistive switching from high resistance state (HRS) to low resistance state (LRS). We examined different types of 2D materials, including 1T MoS_2 and 2H MoS_2 as conductor and semiconductor structural phases of TMDs, graphene and hBN. Here, we illustrate how the electrical conductivity depends on the thickness of the 2D material and its interactions with the electrodes. Additionally, the effect of atomic vacancies and metal ion substitutions on the transport properties is investigated. The defect-induced states within the bandgap, alter the electronic properties and affect the charge transport across the 2D material, thus enabling the resistance switching between LRS and HRS.

References

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

Figures

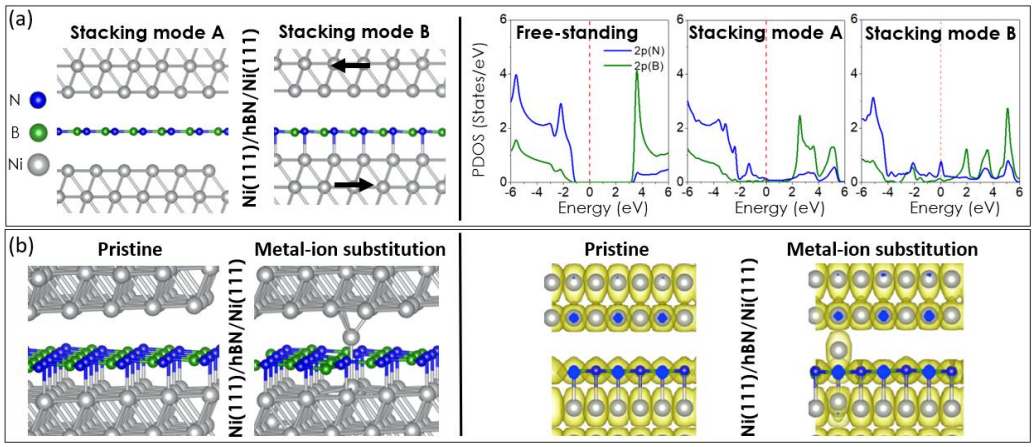

Figure 1: (a) Structural illustration (Left) and density of states (Right) of hBN in different stacking modes. Red dashed line denotes the Fermi level. In stacking mode B, the N-Ni bond formation at the interface induces states within the band gap. (b) Structural illustration (Left) and charge density distribution (Right) of pristine and defected Ni/hBN/Ni systems in stacking mode B. The charge distribution reveals a conductive filament between metallic (Ni) contacts due to metal-ion substitution.

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