Mechanism of Resistance Switching in Hexagonal Boron Nitride

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Resistance switching (RS) is a phenomenon where a material changes its resistance upon application of an external voltage. Hexagonal boron nitride (h-BN) exhibits RS in few or monolayer configurations as well as in bulk-like conditions [1]. The mechanism responsible for the RS effect in h-BN is however still debated. Here, we present a vacancy-driven mechanism that could explain the nonvolatile switching behavior both in bulk as well as in thin h-BN films encapsulated by Au contact. It is supported by *ab initio* device simulations.

The hypothesis that we will demonstrate is that defects can form reversible bonds between adjacent 2-D layers of h-BN [2] and change the conductivity of this material. This is the case of triangular defects, as visualized in Fig. 1. The dependence of the bonding properties of such defects on the charge state is investigated with density-functional theory (DFT) using CP2K [3]. A DZVP basis and the PBE functional is employed for that purpose. First, the forces acting on the neutral configuration of the defect in bulk h-BN are minimized. Then, the charge is decremented in steps of the elementary charge q and the forces minimized at each step. This concept is illustrated in Fig. 2. As the defect charge decreases more interlayer bonds form, up to a maximum of four at $-6q$. Next, the charging is reversed (from $-6q$ to 0), again with force minimizations at each step. During the discharge the bonds remain stable up to the $-3q$ charge state, leading to a hysteresis. Evidently, the charging and discharging of the defect corresponds to the SET and RESET processes of the proposed RS mechanism. The preferred charge state of the defect is shown in Fig. 3 as a function of the Fermi energy. When h-BN is in contact with Au the $2e^-$ and $4e^-$ charge states are preferred at equilibrium, depending on the presence or absence of interlayer bonds. This fact leads to a nonvolatile RS characteristic.

The impact of the defect-induced bonds on the conductance of the h-BN is investigated using a DFT-based quantum transport solver [4]. An Au/h-BN/Au device made of 4 layers of h-BN with a defect is constructed, as drawn in Fig. 4. The electronic conductance is then extracted with the quantum transmitting boundary method (QTBM). The conductance can be seen in Fig. 5, highlighting the presence of a hysteresis as a function of the charge state.

Similarly, bonds can also form between h-BN defects and an Au or graphene contact (Fig. 6). A hysteretic behavior analogous to the one presented here is expected in these cases too. It can therefore be concluded that defect charging is probably at the origin of RS in h-BN.

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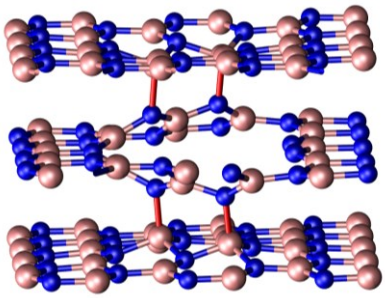

Fig.1: Representation of the atomic configuration of a triangular defect in h-BN where two bonds are formed between the defect and each adjacent layers. The blue and brown spheres represent N and B, respectively, and the interlayer bonds are marked in red.

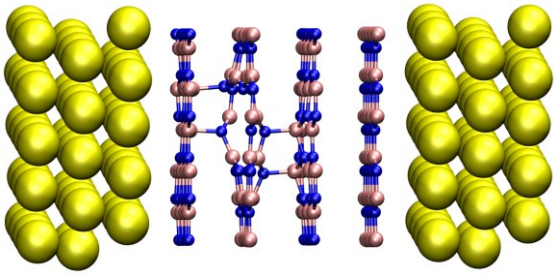

Fig.4: Schematic view of the Au/h-BN/Au structure used to evaluate defect-induced conductance changes. The yellow spheres represent the Au contact atoms. The entire structure is optimized with DFT.

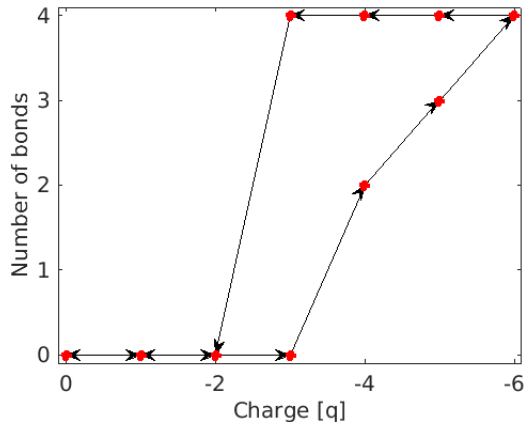

Fig.2: Number of interlayer bonds formed between a defective h-BN layer and its neighbors as a function of its charge. Increasing or decreasing the charge and minimizing the forces may result in a configuration change. Each arrow represents a different step, including a minimization of the force acting on the h-BN structure.

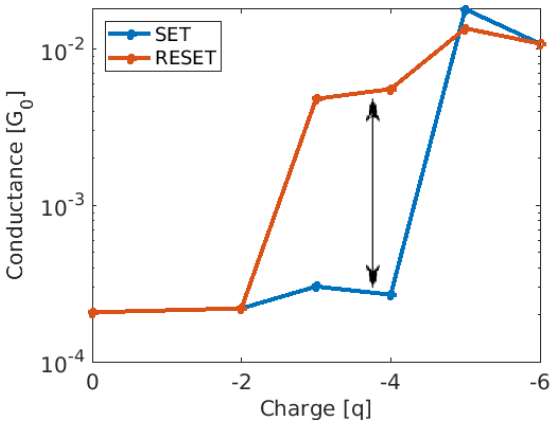

Fig.5: Conductance of the Au/h-BN/Au structure in Fig. 4 as a function of the charge during the SET and RESET processes. States with three or four interlayer bonds are conductive. Hence a hysteresis forms with an ON-OFF conductance ratio of more than one order of magnitude, as indicated by the black double arrow.

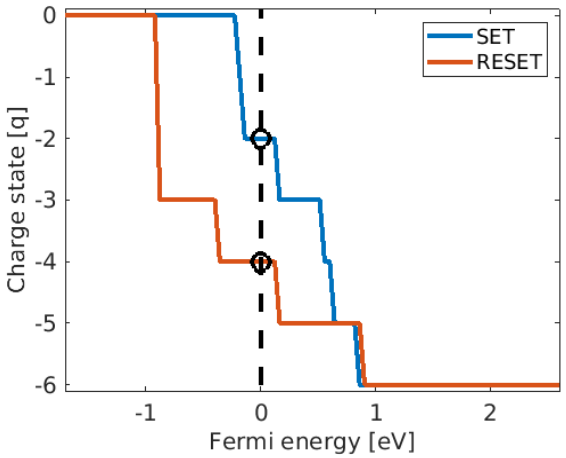

Fig.3: The preferred charge state of the triangular defect as a function of the Fermi energy. The SET and RESET potentials are around 1 eV and -1 eV. These are probably underestimated due to the nature of the PBE functional employed in DFT. The dashed black line indicates the equilibrium potential when the h-BN is in contact with Au. The upper (lower) black circle mark the equilibrium OFF- (ON-) state.

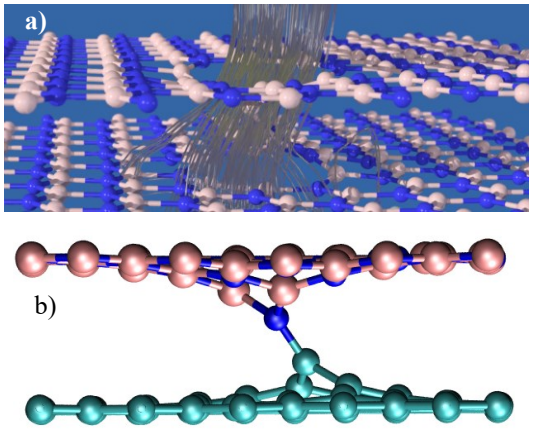

Fig.6: a) The gray lines are an illustration of the current flowing through a defect in h-BN with a single interlayer bond. The pink and blue spheres are the B and N atoms, respectively. b) Example of a defect forming a bond between an h-BN layer and a graphene electrode, where the cyan spheres represent C atoms. The resulting bonding could induce a similar resistance switching characteristic as the one presented here for bulk h-BN.

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