Numerical investigations on 2D materials ferroelectrics for memory devices (2DFERY)

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To develop more efficient nanoelectronic components characterized by low-energy consumption and non-volatile memory, the recent discovery of two-dimensional (2D) materials exhibiting ferroelectric properties, such as SnTe, α-In_2Se_3, and $CuInP_2S_6$, presents new opportunities for miniaturization. The memory device, referred to as a ferroelectric tunnel junction (FTJ), made of a vertical stack of ferroelectric material sandwiched between two metallic contacts, offering the potential for high-density integration and enhanced scalability. Tunnel electro-resistance (TER) ratios that surpass those of FTJs utilizing three-dimensional (3D) ferroelectric materials like HfO_2 have been both predicted and experimentally validated. Furthermore, the improved electrostatic control enables lower power consumption, facilitating polarization switching with reduced voltage requirements.The objective of this project is to investigate various 2D ferroelectric materials in conjunction with different metallic contacts to comprehend the mechanisms underlying these devices and to propose promising material combinations for fabrication and testing. Addressing these challenges necessitates precise numerical simulations. To achieve this, we will adopt an ab-initio approach to study the materials, utilizing Quantum ESPRESSO, a code grounded in Density Functional Theory (DFT), in conjunction with a custom Non-Equilibrium Green's Function (NEGF) formalism to simulate charge transport within the FTJ. This simulation effort, a collaboration between SATIE (DFT) and C2N (NEGF), will concentrate on the α-In_2Se_3 monolayer, as this ferroelectric material is currently under experimental investigation at C2N.This numerical examination of 2D FTJs will yield crucial insights into the transport mechanisms that govern these devices. By assessing the polarization transition mechanisms and the TER of the structures under study, this research will contribute significantly to the design and optimization of non-volatile memory devices based on 2D ferroelectric materials.

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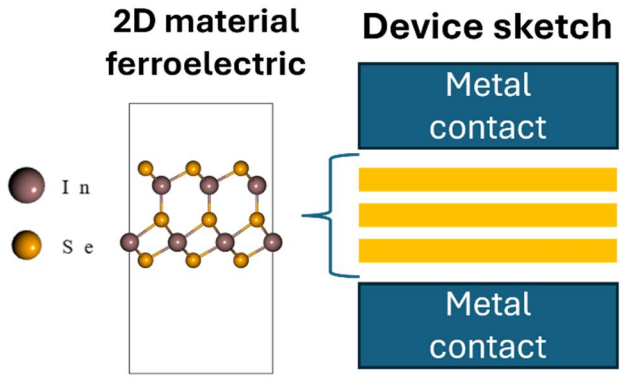

Figure 1 : Sketch of ferroelectric tunnel junction based on 2D ferroelectric material