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Exascale transport simulations for the understanding of the switching mechanism in atomically thin memristors

Non-volatile resistive switching has emerged as an important concept in the development of high-density information storage and computing. The recent discovery of NVRS in two-dimensional (2D) monolayer structures, such as hexagonal boron nitride (hBN), open a new avenue for ultrathin memory/computing devices. The switching mechanism in 2D monolayers, however, is not fully understood. It is hypothesized that vacancies in 2D monolayers mediate formation of conducting filaments leading to a high- to low resistance state. However, questions remain as to why the current on/off ratio and switching voltage are both strongly device-dependent and vary significantly among different experimental works. To address these questions, it is highly desirable to simulate the electronic transport in a realistic device geometry using ab initio approaches for comparison with experimental data. This is rather challenging as quantum transport simulations are computationally demanding. Here, we report results from simulations of electronic transport of ~1000 atom systems consisting of a hBN monolayer sandwiched by gold electrodes and compute I-V curves. These quantum transport simulations are made possible by implementing the non-equilibrium Green's function method in a highly scalable first-principles DFT code: the Real-space MultiGrid (RMG) that runs efficiently in the first exascale supercomputer, Frontier, at ORNL. Systematic calculations reveal that experimental devices exhibit a wide range of on/off ratios due to variations in interface distances between the electrode and h-BN that significantly modulates the gold/h-BN wavefunction overlap. In addition, DFT calculations demonstrate that the energy barrier of a gold atom to dissociate from the electrode and bind with h-BN increases dramatically with the interface distance, thereby explaining the strong dependence of the switching voltage on distance. Our work provides a deeper understanding of the resistive switching mechanism in atomically thin memristors and demonstrates the significance of interface distance in governing the current on/off ratio and switching voltage.

Topical Area

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