

## From Memristor to Spinristor; Endohedral Metallofullerenes for Molecular Electronics

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### Abstract:

Employing multi-scale *in silico* modeling we propose molecular memristors on the basis of endohedral fullerenes, encapsulated with polar molecules of general type MX (M: metal, X: non-metal) to be used for data storage and processing.<sup>[1]</sup> We demonstrate for MX@C<sub>70</sub> systems that the relative orientation of enclosed MX with respect to a set of electrodes connected to the system can be controlled by application of oriented external electric field(s). We suggest systems with two- and four-terminal electrodes, in which the source and drain electrodes help the current to pass through the device and help the switching between the conductive states of the memristor via an applied voltage. The gate electrodes then assist the switching by effectively lowering the energy barrier between local minima via stabilizing the transition state of switching process if the applied voltage between the source and drain is insufficient to switch the MX inside the fullerene. Using non-equilibrium Green's function combined with density functional theory (DFT-NEGF) computations, we further show that conductivity of the studied MX@C<sub>70</sub> systems depends on the relative orientation of MX inside the cage with respect to the electrodes. Therefore, the orientation of the MX inside C<sub>70</sub> can be both enforced (“written”) and retrieved (“read”) by applied voltage. The studied systems thus behave like voltage-sensitive switching molecular diodes, that is a reminiscent of a molecular memristor. Further, we discuss possibility of making a spin-filtering memristor, spinristor, using the similar systems.<sup>[2]</sup>

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### References:

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