Thermal-driven nanofuses based on organometallic mechanical actuators

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INTRODUCTION

Molecular electronics (ME) has attracted an enormous interest in the recent years. Common macroscopic electronic devices, such as wires, resistances, transistors and diodes have now been emulated at nanoscale. Recently, our group has suggested how to reproduce the key characteristics of a nanofuse using an irreversible voltage-controlled *on-off* switching process [1],[2]

In this paper we present a new nanofuse that could run reversibly taking advantage of a mechanical response which connects or disconnects it from bulk electrodes in the presence of a thermal triggering stimulus, i.e. resistive heating, external heating source or electromagnetic radiation.

Our working hypothesis establishes that two different stable states (hereafter *on* and *off* states) connected by a suitable energy barrier (activation energy, E_a) can be turned in the *on-off* sense with the aid of an increase of the thermal energy (Fig. 1). If the molecule has a permanent dipolar moment, a favorable interaction between the molecule and the electric field generated by two electrodes could be used to recover the initial working *on* state. Such dipolar moment should be located in a mobile subunit of the system to interact with the generated electric field. If such dipolar moment is not aligned with the electric field, the mobile subunit undergoes an advantageous torque for the beginning of the fusing event.

The theoretical model has been studied in a truly organometallic compound, a chromium arene (Fig. 2), opening the possibility to the experimental development.

SIMULATION RESULTS AND CONCLUSIONS

Ag (111) electrode surfaces were simulated using a 3×3 cell with periodic boundary conditions, consisting of four layers of 9 atoms using (SIESTA 2.0.2) code. We found the optimal contact distances for nitrile and isonitrile groups of 2.22 Å (E^{ads} = –4.5 Kcal mol $^{-1}$) and 2.0 Å (E^{ads} = –31.0 Kcal mol $^{-1}$), respectively. Computational studies based on Density Functional Theory (DFT) and Non-Equilibrium Green Function (NEGF) approaches provided by Quantum Wise suggest that at low voltage (≤ 0.2 V) the molecule acts as a conductor and the conduction is LUMO controlled (Fig. 3).

In an *on-off* dynamic system, the parameters which have influence on the rate of the switching process are essential data and these parameters have been related with the temperature through the Arrhenius equation, $K = Ae^{-Ea / RT}$. The Arrhenius-type temperature dependence of the system allows the construction of a graphic for selected voltages and the equilibrium constant (Fig. 4). From this graphic we could conclude that the initial *on* state is stable at around 50 K (T_{work}) although an increase in the temperature of 40 K (then reaching 90 K, T_{critic},) switches the system to the *off* state almost instantaneously. The reset event can be also achieved using a reverse voltage pulse of 1 V during only 50 ms.

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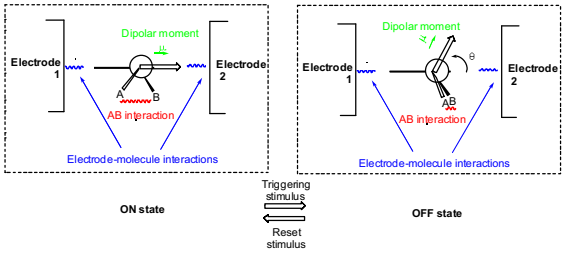


Fig. 1. Working hypothesis of a thermal-driven nanofuse.

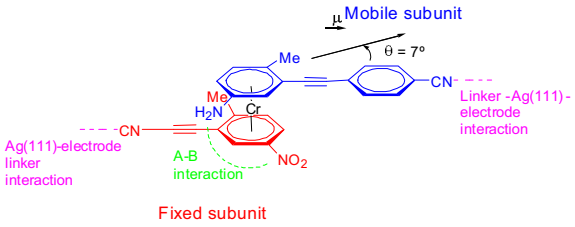
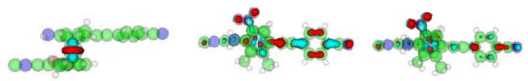


Fig. 2. Chromium arene proposed structure as a model for experimental development.



(a) (b) (c)

Fig. 3. Isosurface plots of the MPSH wave functions at low bias (V = 0) at different energies: (a) HOMO level at –0.43 eV. (b) LUMO level at +0.13 eV. (c) LUMO+1 level at +0.41 eV.

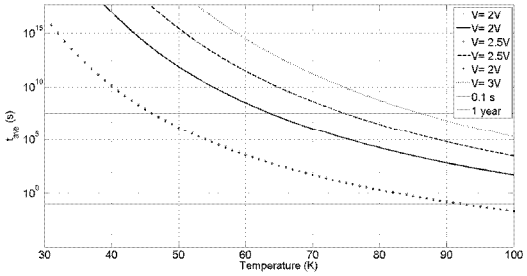


Fig. 4. The Arrhenius-type temperature dependence of the system.