Search for Minimum Molecular Programmable Units*

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Further scaling down of semiconductor devices faces serious obstacles due mainly to device-addressing problems. Practical limitations in fabrication and extraordinary increases in the production costs will also be limiting issues. Small organic molecules, easy to tailor, are the natural alternative to semiconductor components thus giving birth to a completely new area of electronics, molecular electronics or moletronics.

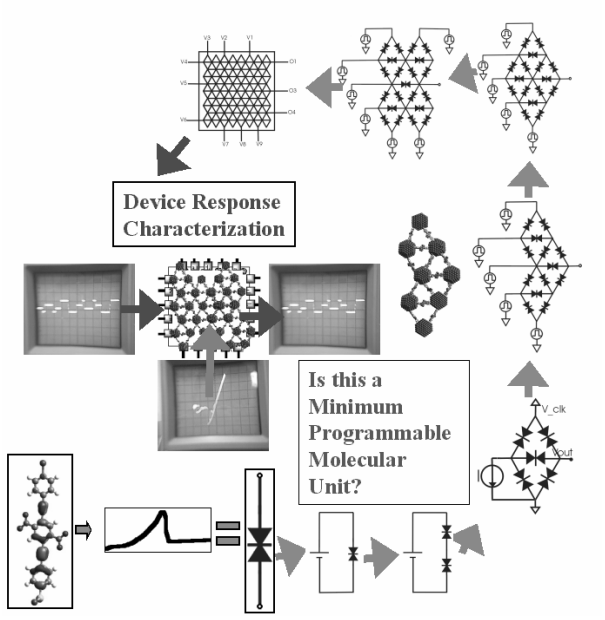

Fig. 1. Design flow for a minimum programmable unit.

We are presenting a summary of our *ab initio* approach to analyze molecular circuits focusing on the development of *field programmable molecular random arrays*. The ansatz that small molecules can be programmed needs to be demonstrated, that means characterizing the smallest molecular system with programmable features as indicated in Figure 1. Current programs for the calculation of current-voltage characteristics of electronic circuits, needed for such demonstrations, are only able to predict single-valued characteristics. We present a procedure to merge molecular physics and quantum chemistry procedures with a practical analysis of molecular *circuits* having strong non linearities. The highly non-linear current-voltage characteristics shown by some molecules open up a complete new set of possibilities for operational circuits, however, the engineering design becomes more complicated and new approaches should be developed since traditional tools for circuit analysis are prepared to deal mostly with linear components. Combination of nonlinear systems yields molecular circuits with multivalued characteristics and determining all the possible states of the circuits is paramount to characterize their operational modes.

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