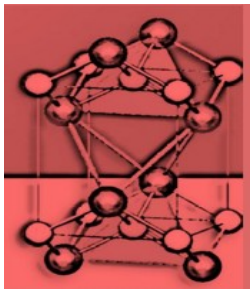

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Understanding mechanisms of ion and electron transport in reconfigurable electrochemical neuromorphic components

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New materials are emerging as promising components of reconfigurable electrochemical random access memory devices. Among them, transition metal oxides such as those containing vanadium, tantalum, titanium, have shown interesting behaviors regarding their abilities to emulate neuronal behavior, including synapses and other neuronal conductance characteristics, which make them potential candidate components for neuromorphic analog computing devices. In parallel, materials based on molecular complexes able to display switchable redox behavior appear as another set of promising components that suitably arranged as molecular films may yield artificial neuronal behavior. Here we analyze the evaluation of ion and electron transport characteristics in these two sets of materials using first principles computational tools, and discuss the fundamental physical and chemical aspects that may drive targeted conductance and memory retention properties. Using first principles theory and simulations we highlight similarities and differences between these two sets of materials regarding their conductance properties and neuromorphic behavior.