To develop a nanostructured switching material that is based on molecular conformational switching as a state variable. Individual switches are electrically addressable and are able to store information. The molecular state can be read at high rates with virtually no dissipating energy by short wavelength optical methods.

Quantum mechanics has been used extensively to interpret, design and develop molecular electronic systems. In particular the Goddard group has designed quantum mechanical simulation tools that have been shown to accurately predict dynamic processes in electro active molecules. Certain organometallic complexes are known to have different conformations in different oxidation states. Copper for instance undergoes a conformational change for tetrahedral Cu(I) reduced state to square planar Cu(II) oxidized state. These types of copper systems will be implemented as rotors in the switches described herein.

Density functional theory (DFT) calculations were performed using Jaguar ver 7.5. Geometry optimizations were carried out using the M06 functional. In order to validate our method against experimental results, we estimated reduction potentials at standard conditions ($E^0$) for Cu(I) and Cu(II) with bisphenathroline (phen) and 2,9-dimethyl-1,10-phenanthroline (dmp) ligands in acetonitrile.

We have identified that only Copper (bisphenantroline) and (3,8-bispropilydinephen) complexes present higher reorganization energy and molecular motion. We also performed calculations on Cu phenantroline with a bidentate stator.

DFT is able to accurately predict solution oxidation potentials. We performed a theoretical study on the conformational changes of Cu phenanthroline complexes. Our results confirm that unhindered (2,9-unsubstituted) phenanthrolines undergo significant geometrical changes upon electron transfer. The addition of a phosphine-based stator increases the reorganization energy $\lambda$. This is beneficial since there is more energy available to perform rotational work when the complex is oxidized.

In the future we will screen a series of potential rotators and bidentate stators. We will evaluate the systems with the parameter $\lambda$. Several metals including Ru, Fe, Zn with several ligands will be evaluated as useful experimental controls. We also will carry out dynamics of the switching mechanism on surfaces, using hybrid quantum and classical mechanical methods.