Nanoelectronic Switches

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER

***Objective*: Explain the cause of reversible binary switching in a mechanically-controlled, single-molecule junction.**

***Implications*: Possible basis for a new class of switches useful for electronics. Key synergy between NERSC and LBNL Molecular Foundry.**

***Accomplishments:* Density Functional Theory reveals the bonding mechanism in the molecule that spans the junction.**

- **Shows conductance to be directly related to degree of tilt and type of molecule.**
- **Total of 55 different junction configurations studied.**

***NERSC:* High throughput and power of the NERSC resources facilitated a highly interactive back-and-forth with experimentalists.**

- **PWscf, Paratec, SCARLET Codes, typically 100-500 cores**

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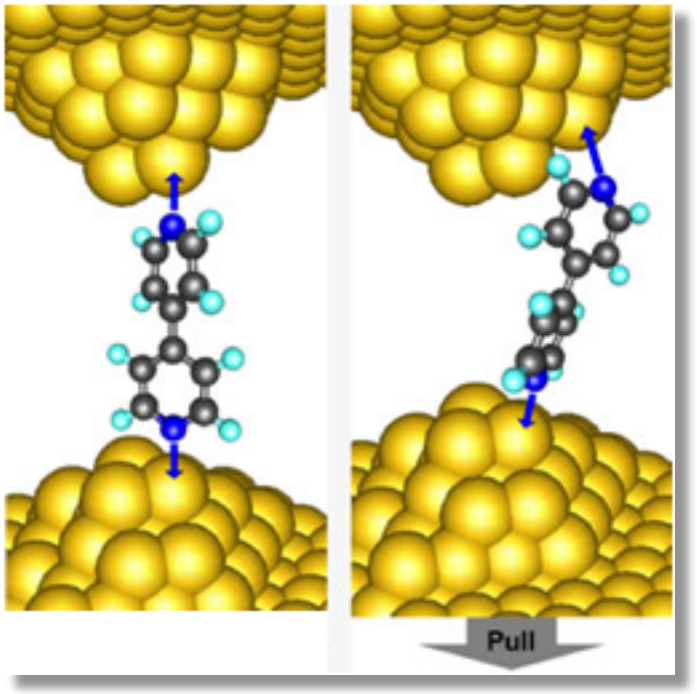

Schematics showing the molecular junction configurations for a model nanoswitch based on a junction between gold electrodes and a bipyridine molecule that is either vertical or tilted.

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