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Mechanism of Current-Induced Switching in Naphthalocyanine Molecular Device TESHAYE ABTEW, NC State U. Raleigh NC, JERRY BERNHOLC, WENCHANG LU, NC State U. Raleigh NC and CSMD, ORNL, TN — Current-induced switching of inner cavity hydrogen atoms in a naphthalocyanine molecule has been reported experimentally [1]. The experiment shows a rotation of the lowest unoccupied molecular orbital (LUMO) image by 90° when the switching occurs. We study transport properties and energetics of a naphthalocyanine molecule sandwiched between gold leads using a parallel real space multigrid method. A non-equilibrium Green's function formalism in a basis of optimized localized orbitals is employed to evaluate the current-voltage characteristics. Current-induced forces are evaluated and used to obtain bias-induced relaxations. The current-voltage characteristics indeed reveal contrasting high and low conductances depending on the orientation of the hydrogen atoms. However, a high energy barrier restrains the hydrogens from switching. We propose an alternative atomic configuration, which yields a much lower energy barrier for switching but still results in LUMO images that agree with the experimental results. [1]. P. Liljeroth, J. Repp, and G. Meyer, *Science* 317, 1203 (2007).

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