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First-principles studies of the switching performance of [2]rotaxane molecules and monolayers KINYIP PHOA, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley, J.B. NEATON, The Molecular Foundry, Materials Sciences Division, Lawrence Berkeley National Laboratory, VIVEK SUBRAMANIAN, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley — Density functional theory calculations of [2]rotaxane, an organic molecule consisting of a linear (straight) backbone and an encircling ring, which was recently proposed as the basis of a molecular memory device[1], are presented. The energy landscape describing the shuttling of the ring along the backbone is calculated and carefully investigated. Furthermore, to estimate the potential RC delays associated with this molecular memory circuit, the long-wave dielectric response of [2]rotaxane monolayers is explored by applying an external field. Our calculations shed new light on the underlying working principle of this system and build on previous studies[2].

[1] Y. Luo, et. al., ChemPhysChem, 3, 519-525, 2002
[2] Y. H. Jang, et. al., J. Phys. Chem. B 110, 7660-7665, 2006

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