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Molecular switch modifications by single atom manipulation M. MAMATKULOV, L. STAUFFER, PH. SONNET, LPSE, 4, rue des Freres Lumiere 68200 Mulhouse, France, M. MARTIN, M. LASTAPIS, D. RIEDEL, G. DUJARDIN, LPM, Bat 210 Universite Paris Sud 91405 Orsay, France — The operation of a single molecule as a molecular nanomachine requires controlling the interaction between the molecule and its surrounding with an atomic scale precision. Recently, it has been demonstrated that a single biphenyl molecule adsorbed on a Si(001) surface behaves as bistable molecule at low temperature. By means of ab-initio calculations, we study the underlying physics of this system. A variety of configurations for the adsorbed biphenyl molecule have been investigated [1]. We show that, during its adsorption on Si(001), one hydrogen atom dissociates from one phenyl and bonds to a neighbouring surface silicon atom. After desorbing this hydrogen with a STM tip, the dynamics of the adsorbed biphenyl molecule is strongly modified: it becomes a multistable molecule having four stable states. Local density of states calculations have been performed and compared to the experimental STM topographies. A good agreement has been observed, allowing a deeper understanding of this system [2]. Our study emphasizes that, by means of a single atom manipulation, one expect to be able to control the intrinsic performance of molecular device. [1] M. Mamatkulov et al., Phys. Rev. B 73 (2006) 035321 [2] M. Martin et al., Phys. Rev. Lett (accepted)

Mikhail Mamatkulov
LPSE, 4, rue des Freres Lumiere 68200 Mulhouse, France

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