Molecular switch modifications by single atom manipulation

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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
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