Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Tunneling and Time-Reversal Invariance in the Diffusion of Polyatomic Molecules at a Metal Surface ZHIHAI CHENG, ERIC CHU, DEZHENG SUN, DAEHO KIM, YEMING ZHU, MIAOMIAO LUO, GREG PAWIN, KIN WONG, KI-YOUNG KWON, ROBERT CARP, MICHAEL MARSELLA, LUDWIG BARTELS, UCR — Rectangular molecules with 1 or 2 oxygen substrate linkers attached to each of their long sides diffuse in a uniaxial fashion, despite the threefold symmetry of the Cu(111) substrate. They achieve this by sequential placement of their substrate linkers and are hence dubbed "molecular walkers". VT-STM monitoring of their motion reveals a striking difference between the diffusion prefactors of the quadrupedal and bipedal species, with the latter being very low. DFT modeling of the diffusion barrier and WBK-based estimation of the potential for tunneling suggest that this discrepancy lies in the prevalence of tunneling for species, whose motion is only blocked by a barrier affecting one of their substrate linkers. In contrast, if the diffusion barrier affects two substrate linkers simultaneously, tunneling will not occur and conventional prefactors are observed. This finding may actually have far-reaching implications for the modeling of molecular motion in general, as it highlights that blocking of a single atoms is insufficient for confinement of molecular motion. We also investigated an asymmetric "molecular walkers", showing a symmetric diffusion in agreement with time-reversal invariance despite a saw-tooth shape of the diffusion barrier experienced.

Theodore Einstein

Date submitted: 27 Nov 2010 Electronic form version 1.4