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On the track of nano-vehicles: A Molecular Dynamics Approach

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Abstract – We have performed atomistic molecular dynamics simulation of a variety of molecules from the class of nanocars (three-wheeled nanocar and nanotruck) as synthesized by the J. M. Tour's group. We used different force fields and charge protocols to investigate how the results are method dependent. The explicit inclusion of a simulated STM tip produced results consistent with the experimental data and might explain some inconsistencies between theory and experiments reported in the literature.

Recent advances in experimental techniques, for both imaging and molecular synthesis, has led to significant progresses in the design of a variety of single-molecule-sized nanomachines, such as; vehicles, shuttles, gears, bearings, etc. [1]. Carbon-based nanocars and trucks were synthesized by J. M. Tour's group [2]. They consist of two up to four fullerene wheels and an organic structure acting as chassis and rotational axles. The experimental studies consisted of depositing the molecules over gold surfaces and analyzing their dynamics from STM experiments. A realistic computational simulation of these experiments is very difficult. Recently, Akimov et. al. [3] reported a molecular dynamics (MD) study using simplified molecular models. Although some experimental aspects were well reproduced, others are in clear disagreement with the experimental data. The origin of these discrepancies remains to be explained.

We have reinvestigated these problems using different computational tools trying to mimic the experimental conditions. We have carried molecular dynamics simulations using both reactive force field as implemented in the ReaxFF code [4], and non-reactive force fields. We have also used a density functional theory-based tight binding method (DFTB+) [5]. For the simulations the following structures were investigated: three-wheeled nanocars and a nano-truck [1, 2]. Also, in order to estimate the relative importance of the substrate, energy profiles of molecular movements over Au(111) were calculated. The molecular dynamics simulations were performed at temperatures from 50 up to 600K. Different charge distributions applied to the system were used. Our results show that a point charge moving relative to the surface is able to induce molecular movements along tip direction (Fig. 1). This approach, though simplified, explicitly incorporates the effect of STM tips used in the experiments, which might explain some of the observed discrepancies between experiment and previous simulations [3].

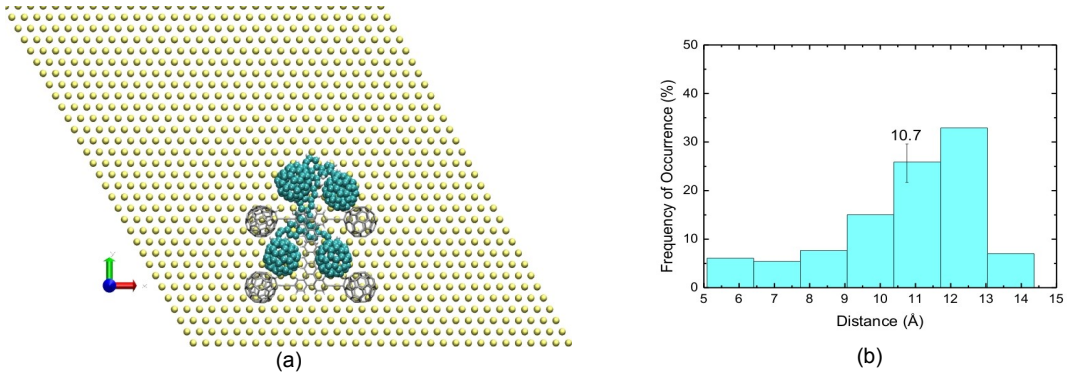

Figure 1: Simulated car dislocation over Au (111) due to electric field from the STM tip. (a) Top view of the first (gray) and last (cyan) frames of the MD simulations; (b) Distribution of truck's atomic displacement, where 10.7 Angstroms indicate the centroid dislocation.

References

[1] Y. Shirai, et. al., Nano Lett. 5, 2330 (2005)
[2] Y. Shirai et. al., Chem. Soc. Rev. 35, 1043 (2006).
[3] A. V. Akimov et. al., J. Chem. Theory Comput. 4, 652 (2008).
[4] A. C. T. van Duin, S. Dasgupta, F. Lorant, and W. A. Goddard III, J. Phys. Chem. A 105, 9396 (2001).
[5] http://www.dftb-plus.info/