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A study of Rolling Mechanism of Single molecule on Metal surface

MELIHAT MADRAN, Sabanci University, ALIMET ZEN, ZEHRA AKDENIZ, piri reis university, SONDAN DURUKANOGLU, Sabanci University — We present the results of DFT and molecular dynamic calculations for wheel dimer molecule on corrugated Cu(110) surface. We examined all possible configurations of $C_{44}H_{26}$ with respect to substrate based on calculations with the vDW-D2 and PBE functional to compare with the experimental results and to better understand the role of van der Waals interactions on the adsorptions of wheel dimer molecule. We also performed molecular dynamic calculations to investigate how the temperature of the system plays roles on the configurations of the molecules on Cu(110) surface. Furthermore, to identify the behavior of molecular motions on corrugated metal surface in the existence of STM tip, we looked deeper into the position of STM tip with respect to central molecular axle during the molecular dynamic simulations. Using the results of MD simulations in the existence of STM tip, we further discussed the position of STM tip for rolling mechanisms of wheel dimer molecule on Cu(110) surface.

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