Seminář odd. 26
Tenkých vrstev a nanostruktur

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TÉMA

SELF-ASSEMBLY OF AZAHELICENES ON AG(1,1,1): STM AND COMPUTATIONAL STUDY

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We studied self-organization of azahelicenes ((+)-(P)-2-aza[6]helicene) on Ag(1,1,1) surfaces. Combined scanning tunneling microscopy (STM) and tuning-fork-based noncontact atomic force microscopy (NC-AFM) were used to explore the system experimentally. Regular flower-like cyclic aggregates consisting of six azahelicenes were observed. Computational chemistry methods were then applied to estimate the structure of the observed molecular clusters. Density functional theory calculations with empirical correction for the dispersion interactions (bp86/def2-SVP) and molecular dynamics simulations using the TINK code with Universal Force Field were employed to calculate the Ag(1,1,1)-azahelicene complexes and interpret the experimental results. Calculated structures are shown in Figures 1 and 2. The latter Figure also demonstrates the agreement with the STM image.

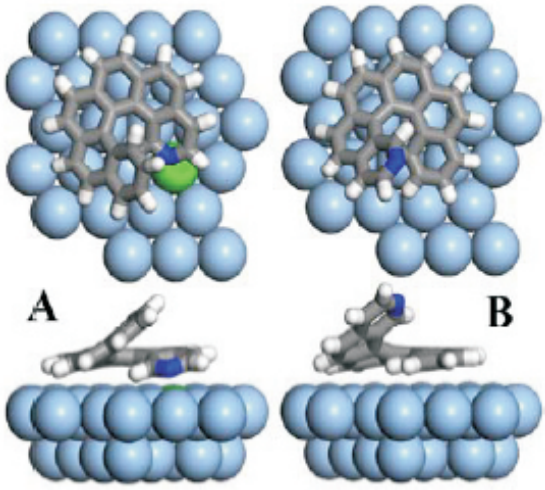

Figure 1. Optimized geometries of ((+)-(P)-2-aza[6]helicene on Ag(1,1,1) surface.

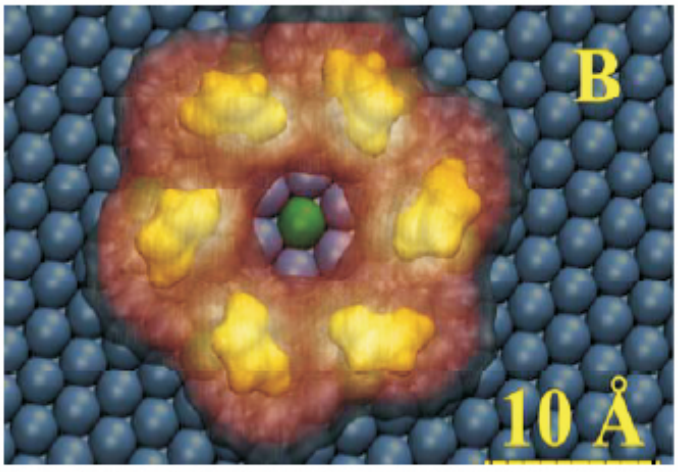

Figure 2. Superposition of the STM observed aggregate and a structure from the molecular dynamics simulation.

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