

Advanced Materials 2019: The unit cell prediction of two-dimensional supramolecule by STUN-BH-DMD method and molecular dynamics simulation- Tsu-Hsun Hou- National Sun Yat-sen University

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The unit of two-dimensional STA supramolecule on a virtual graphene surface was predicted during this study. The DREIDING field was used to describe the interatomic interactions and therefore the Electrostatic Surface Potential (ESP) charges obtained by the semi-empirical initially package VAMP with the NDDO (Neglect of Diatomic Differential Overlap) Hamiltonians approximation method of PM6 (Parameterization Method 6) was used for the DREIDING potential. First, the Stochastic Tunneling-Basin-Hopping-Discrete molecular dynamics method (STUN-BH-DMD) was used to predict the foremost stable STA layer on the virtual graphene surface. The box shape was adjusted during the STUN-BH-DMD search process and therefore the ordered unit of STA supramolecule was predicted. The molecular dynamics simulations were used to investigate the thermal stability and diffusion behaviors of STA supramolecule. The energy-temperature profiles were used to pinpoint the temperatures, at which the STA supramolecule structure begins damaged and therefore the mean-square displacement profiles were used to investigate the dynamical behaviors of STA supramolecules at different temperatures also as deriving the diffusion coefficients of STA.

The molecular structure and dynamics at the interface between a sheet surface and a liquid is of considerable interest, e.g., within the context of lubrication, adhesion, molecular recognition phenomena at interfaces, or for the organization of

molecules possibly undergoing topochemical reactions. Recent scanning tunneling microscopy (STM) studies at the interface between organic solutions or melts of long chain alkanes and straightforward alkyl derivatives and therefore the basal plane of graphite reveal highly ordered lamellar structures. The STM images confirm an earlier model proposed on the idea of adsorption isotherm and enthalpy measurements. It suggests that over a substantial range of concentrations the solute molecules physisorb in all-trans conformation parallel to the surface, forming densely packed monolayers. A detailed analysis of the STM results allows, additionally, to determine the commensurability between substrate and adsorbate lattices, both along the molecular axes of the adsorbate also as along the lamellae. The time resolution of the STM experiment, however, is restricted to the millisecond duration. While this is often sufficient to watch the cooperative reorganization of a couple of molecules within the monolayers, it is way too slow to observe the intramolecular dynamics in this case. Here we combine STM results with computer simulations to get further insight. Computer simulations are now among the quality theoretical approaches to adsorption phenomena on solid surfaces. Methods like Monte Carlo or molecular dynamics (MD) are useful tools in the study of the translational and orientational ordering of adsorbates, their commensurability or incommensurability with the substrate, the dynamics of adsorbates, and therefore the universal and nonuniversal aspects of surface phase transitions.