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The unit cell prediction of two-dimensional supramolecule by STUN-BH-DMD method and molecular dynamics simulation

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The unit cell of two-dimensional STA supramolecule on a virtual graphene surface was predicted in this study. The DRIEDING force field was used to describe the interatomic interactions and the Electrostatic Surface Potential (ESP) charges obtained by the semi-empirical ab initio 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 most stable STA layer on the virtual graphene surface. The box shape was adjusted during the STUN-BH-DMD search process and the ordered unit cell 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 the mean-square displacement profiles were used to investigate the dynamical behaviors of STA supramolecules at different temperatures as well as deriving the diffusion coefficients of STA.

Biography

Tsu-Hsun Hou is currently pursuing Master's degree at National Sun Yat-sen University in Kaohsiung, Taiwan. In recent years, he has been particularly engaged in the research of metal high-entropy alloys, biomolecules, polymers, supramolecules and so on. He has also worked with a number of medical research institutions and through both the experimental and the analog end of the collaboration, research efficiency can be greatly improved.

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