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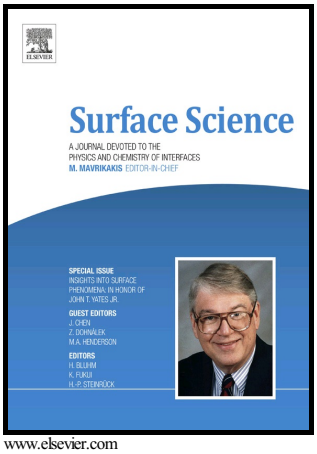

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Development of simulation approach for two-dimensional chiral molecular self-assembly driven by hydrogen bond at the liquid/solid interface

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Abstract

Two-dimensional (2D) chiral self-assembly system of 5-(benzyloxy)-isophthalic acid derivative/(S)-(+)-2-octanol/highly oriented pyrolytic graphite was studied. A combined density functional theory/molecular mechanics/molecular dynamics (DFT/MM/MD) approach for system of 2D chiral molecular self-assembly driven by hydrogen bond at the liquid/solid interface was thus proposed. Structural models of the chiral assembly were built on the basis of scanning tunneling microscopy (STM) images and simplified for DFT geometry optimization. Merck Molecular Force Field (MMFF) was singled out as the suitable force field by comparing the optimized configurations of MM and DFT. MM and MD simulations for hexagonal unit model which better represented the 2D assemble network were then preformed with MMFF. The adhesion energy, evolution of self-assembly process and characteristic parameters of hydrogen bond were obtained and analyzed. According to the above simulation, the stabilities of the clockwise and counterclockwise enantiomorphous networks were evaluated. The calculational results were supported by STM observations and the feasibility of the simulation method was confirmed by two other systems in the presence of chiral co-absorbers (R)-(-)-2-octanol and achiral co-absorbers 1-octanol. This theoretical simulation method assesses the stability trend of 2D enantiomorphous assemblies with atomic scale and can be applied to the similar hydrogen bond driven 2D chirality of molecular self-assembly system.

Graphical abstract