Molecular dynamics study of polarized C60 on an organic surface

QIANG LIU, WEI JIN, JOHN D. WEEKS, JANICE REUTT-ROBEY — The experimental results of vapor deposition of C60 on a variety of organic molecular films has showed unusual meandering chain structures. Here we use the Langevin molecular dynamics method to mimic the system. In the simulation, we considered interactions including the intermolecular Girifalco potential, dipole-dipole interactions, octupole interactions suggested by W. Losert and substrate potentials. Choosing different parameters can give us different C60 patterns: the close-packed C60 islands, isolated C60 molecules and meandering chain islands.

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