금(111) 표면에 흡착된 부탄싸이올의 구조와 에너지 계산

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First-principle calculations of adsorption structure and energies for butanethiol on the Au(111) surface

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Key Words: SAM(자기조립 단분자막), Au(111)(금(111)표면), butanethiol(부탄싸이올)

Abstract : The adsorption of butanethiolate on the Au(111) surface have been investigated by first-principle calculation. In order to see a chain length effect, we also considered an adsorption of decanethiolate and methanethiolate using pseudopotential and LCAO methods within DFT. To establish the reliability of the present methods, we performed test calculations for gold(atom, bulk, slab) and small molecules of various combinations of S, C, and H. Stable adsorption geometries and adsorption energy of thiolate on Au were obtained..This study provides some insight for the interactions involved with thiols and gold surfaces in Microcontact printing(μCP) and dip-pen nanolithography(DPN) which use "gold paper"-"thiol ink". The effort to link present results to physical parameters necessary to simulate such nanoscale processes is underway.

양극성 계면활성제에 의해 표면 전도도가 조절된 탄소나노튜브에 대한 유전영동

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Dielectrophoresis of surface conductance modulated Single-walled carbon nanotubes using catanionic surfactants

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Key Words: Single-walled Carbon Nanotubes(단일벽 탄소나노튜브), Dielectrophoresis(유전영동), Surface Conductance(표면 전도도), Catanionic Surfactant(양극성 계면활성제)

Abstract : Dielectrophoresis has received considerable attention for separating nanotubes according to electronic types. Here we examine the effects of surface conductivity of semiconducting single-walled carbon nanotubes (SWNT), induced by ionic surfactants, on the sign of dielectrophoretic force. The crossover frequency of semiconducting SWNT increases rapidly as the conductivity ratio between the particle and medium increases, leading to an incomplete separation of ionic surfactant suspended SWNT at an electric field frequency of 10 MHz. The surface charge of SWNT is neutralized by an equimolar mixture of anionic surfactant sodium dodecyl sulfate (SDS) and cationic surfactant cetyltrimenthylammonium bromide (CTAB), resulting in negative dielectrophoresis of semiconducting species at 10 MHz. A comparative Raman spectroscopy study shows a nearly complete separation of metallic SWNT.