Theoretical Study on Morphology of Copper Sulfide via Density Functional Theory Calculation

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Copper sulfide has been attracted attention as a well-known p-type semiconductor because of low cost of precursor and its vast potential applications including photothermal therapy, optoelectronics, catalysis, and battery. The control of morphology is also critical influence factor to change their physical, optical, and chemical properties. In this study, the crystal growth and morphological changes of copper sulfide were studied by density functional theory (DFT) calculations. In particular, since one-dimensional (1D) nanoparticles including nanofiber, nanowire, and nanorod and two-dimensional (2D) such as nanoplate, and nanosheet have been experimentally synthesized, the DFT calculations have focused on both types. Especially, the CuS morphology was calculated as a hexagonal plate, through the stacking energy calculation of each surface, and morphological change to 1D structure were estimated according to the interaction with each surface with the surfactant. In addition, morphological changes were also observed depending on surfactant type because the interaction with each surface was different depending on the type of surfactant.