Morphology Control of Zinc-blende Nanocrystal Structure by Oleate Depending on Temperature

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The electronic, optical, and catalytic properties of nanocrystals (NCs) are highly dependent on NCs morphology. It is therefore of great importance to control the morphology of NCs. The NCs morphology can be changed due to several factors including temperature, ligands, and colloidal composition, etc. In this study, density functional theory calculations were performed considering the zinc-blende ZnSe structure with oleate as a X-type ligand depending on temperature. The equilibrium morphology was obtained by the Wulff construction, which minimized the surface energy for a given volume. Morphologies of ZnSe NCs were obtained by varying the temperature from 0 to 600 K. The Gibbs free energy of binding of oleate on the (111) surface was the highest, hence the tetrahedral-shaped NC with all facets of the (111) surface was observed. As the temperature increases, the (220) surface begins to appear in the equilibrium morphology since the increase in surface energy of (220) is the slowest among other surfaces. Through the theoretical model considering the surface-ligand interaction, we scrutinized the relationship between the temperature and NCs morphology.