

ELECTRON STRUCTURE OF AGCL NANOCRYSTAL WITH SILVER ION ADSORBED ON ATOMICALLY ROUGH SURFACE

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Using semi-empirical tight-binding technique applying self-consistency over effective charges and dipole moments of the ions total and local density of states were calculated for AgCl nanocrystals with the adsorbed silver ion. Adsorption was considered as on atomically rough surface (near the step and step fracture) as on the smooth surface. Basing on the obtained data one can make a conclusion that an increase of photoelectron localization can be expected with a decrease of the number of anions in a substrate that is the nearest ones to the adsorbed ion. It means that the most efficient photoelectron capture has to take place under adsorption on the smooth surface rather than near the steps and their fractures as it was previously assumed.