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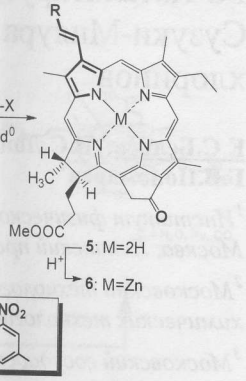
Дифракционные методы в характеризации новых материалов

Труды симпозиума

31 мая – 2 июня 2017 г.
Москва, Россия



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Study of Electronic Density for the Case of Silicon Nanocrystals Stabilized with Phenyl and Perfluorophenyl Ligands

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Recently the series of syntheses of Si nanocrystals stabilized by different ligands have been performed in different organic solvents [1]. As a result the isotropic quantum dots have been obtained except the case when Si nanoparticle was covered by perfluorophenyl ligands. In this case flat silicon nanoparticles have been obtained. The size of these particles varied from 15 to 50 nm. Their thickness evaluated with the atomic force microscopy was about 3.3 nm.

We used ab initio DFT calculations to investigate the geometries and electronic structures of free standing perfluorophenyl stabilized 2D silicon structures in order to see if such systems have promising electronic and optical properties [2]. The interesting question is the difference in electronic density configurations for the quantum dot (we take stabilization by phenyl ligands for this case) and 2D structure cases.

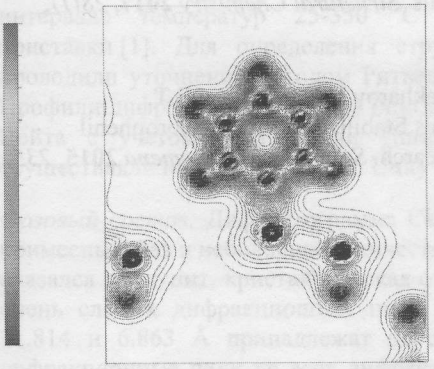

Figure 1. Fragment of SiPh valence density in the film geometry.

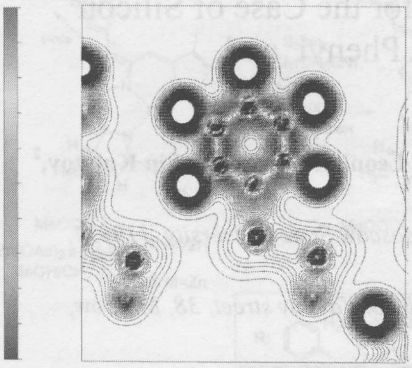

Figure 1. Fragment of SiFPh valence density in the film geometry.

In this report we present ab initio investigation of electronic density for these two cases (see fig.1 and fig.2). We analyze the electronic density properties and discuss the self-assembling mechanism in the perfluorophenyl case.

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References

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(2) Aslanov L.A., Kudryavtsev I.K., Zakharov V.N., Kulatov E.T. Free-standing Flat Silicene Nanocrystals Stabilized with Perfluorophenil Ligands: Experiment and ab initio Research. *Solid State Phenomena* **2015**, *233*, 575-578.