

# Simulation of molecular structure and electrical conductivity of metal phthalocyanines as the basis of the self-assembly monolayers

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Layer-by-layer assembly method is widely used for the creation of ultra-thin organic films. This method solves the problem of creating layers with specified properties that include molecules oriented in definite direction relative to each other and the substrate. One variation of the layer-by-layer assembly method is the polycation/polyanion self-assembly. It allows you to receive a variety of polymer coatings that are used extensively to create new generation devices. Synthesis of molecules with pre-defined structure is promising for manufacturing the various organic electronics materials [1].

Layer-by-layer assembly method is also used for adsorption of organic semiconductors, for example, based on metal phthalocyanine molecules [2]. Organic semiconductors based on metal phthalocyanine molecules are photosensitive and, therefore, are used to make solar cells, photovoltaic cells and other electronic devices. Photovoltaic cells are used in optical fiber of communication systems, measurement technology and energy industry [3]. Phthalocyanine dyes are also used to create new generation displays, as these dyes exhibit nonlinear optical properties [4] and optical memory [5].

The aim of our work is the simulation of molecular structure properties and electrical conduction through metal phthalocyanines and polyelectrolytes implementing Gaussian 09[6,7] software. In particular, we have calculated molecule's conformation, binding energies and their alterations under illumination as well as charge transfer through the film. The copper phthalocyanine (CuPc) and hydroxy-aluminum trisulphonated phthalocyanine (AlPcS) complexes have been studied. Geometry optimization of metal phthalocyanine molecules has been performed by density functional theory (DFT) using B3LYP theoretical model and the standard 6-311G basis set.

As a result, the quantum chemical simulations of metal phthalocyanines confirm the fact of illumination-driven alteration of their adsorption properties, however, only for nonsymmetrical molecules (AlPcS), not for symmetrical ones (CuPc). The following explanation of this fact is proposed: illuminating the nonsymmetrical phthalocyanine molecule increases its AlPcS dipole moment and thereby enhances its hydrophilicity that facilitates molecule's adsorption onto PEI layer.

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