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Donor-Acceptor Dyads Monolayers and Their Structural Investigation

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Abstract:

Ever since porphyrin-fullerene dyad [1] composed of fullerenes (acceptors) and porphyrins (donors) had been successfully synthesised and investigated for the first time, they had attracted a considerable attention of the researchers as efficient molecular systems for photoinduced charge separation. For practical use in photovoltaic devices and biochemical sensors the dyad molecules must be organized into layer structure with the uniform orientation order of donor-acceptor pairs. A convenient method of obtaining such organized structure is Langmuir technique. It requires surface-active compounds and is based on self-assembling of such compounds at the water-air interface. It was shown that dyads could be deposited onto solid substrates, and the orientation of dyads in the film was confirmed by the time resolved Maxwell charge displacement measurements of the photovoltaic response of the samples [2].

In present work the monolayers of porphyrin-fullerene dyads (TBD6a, ZnDHD6ee, DHD6ee) were formed on the surface of water subphase and transferred onto a solid substrate by Langmuir-Schaeffer method.

The structures of isolated molecules and their packing in accordance with the data of area per molecule isotherm were built using computer modeling methods.

The research of structural properties of molecular films on the substrate had been done by X-ray reflectometry method. Orientational properties of dyads were studied by X-ray standing waves method in the region of total external reflection. The crystal structure of organic monomolecular films was studied by electron diffraction. The experimental data had been compared with the results of molecular modeling of the single molecules, to clarify the structure of monolayers and modeling of electronic properties of the investigated systems.

As a result of the research the data on structural properties of monolayers of porphyrin-fullerene dyads were obtained. The thickness of the monomolecular layers and the orientation of organic molecules on the surface of the solid substrate was determined. was determined. An analysis of the diffraction patterns showed also that 3D microcrystallites can be formed in some regions of films during their transfer. It is shown that the deposition of the monolayer onto a silicon substrate inherits dyad orientation on a water subphase surface, that is in good agreement with the photovoltaic response of such structures [3].

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