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Simulation on morphology controlling additives on Pigment Yellow 181, $C_{25}H_{21}N_7O_5$

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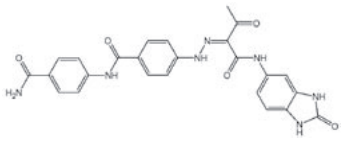
Pigment Yellow 181 is an industrially important reddish yellow pigment. The pigment usually crystallizes in thin needles. With a special additive a plate-like morphology can be obtained. [1] The platelets are arranged into a porous microsphere structure. Molecular modelling was used to study the influence of the additive on the pigment morphology. The adsorption enthalpies of a fragment of the additive on several crystal faces were calculated. The calculations show that the additive adsorbs preferably on one face and also blocks the growth in the needle direction. In consequence the pigment crystallizes not in thin needles but in plates.



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Keywords: pigments, morphology, molecular modelling

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A theoretical study of changes in the morphology of the diarylethene crystals

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The photochromic molecules, diarylethene and its derivatives, show reversible transformation by photoirradiation between two states that have different absorption spectra. Hence, such molecules have considerable potential to work as molecular devices, such as the molecular switch and memory[1]. Recently the dynamic changes in the morphology of diarylethene crystals were reported. It was found that surface morphology of the crystal can be reversibly changed by alternate irradiation with ultraviolet and visible light[2]. The photochromic reaction mechanism in the crystalline phase of diarylethene has been widely studied by using X-ray crystallographic analysis, solid state NMR and AFM. In this work, we further characterize the photochromic reaction of diarylethene and its derivatives with a theoretical study on the crystal properties. The reproduction of the known crystal structures (open- and closed-ring forms) by lattice energy minimization was carried out using DMAREL[3] with distributed multipoles derived from *ab initio* calculations. The good agreement between the optimized and measured crystals confirms the adequacy of the potential model for this study. We then applied this theoretical model to the elastic constant calculations for both photogenerated isomers (open-ring and closed-ring forms). The influence of the elastic anisotropy on the morphologic changes of the diarylethene crystals during the photochromic reaction was discussed.

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Image reconstruction by a combination of diffractive imaging and selected area nano diffraction

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Diffractive imaging is one of the novel methods for obtaining structural information in the real space from diffraction patterns. The notable merit when applying this method to electron diffraction is that image contrast and spatial resolution in the reconstructed images are not limited by lens aberrations in TEM. To reconstruct images by the diffractive imaging, boundary conditions in the real and the Fourier spaces are combined consistently by iterative optimisations through Fourier transforms. The boundary condition for electron exit wave fields in the real space is that the amplitude must be a constant value in areas where no material exists. The condition means that the diffractive imaging can be applied only to samples in isolated shapes like carbon nanotubes [1]. To avoid the restriction, we propose a new method applicable to samples in arbitrary shapes by using the selected area diffraction (SAD). In the new method, a region where electron beams are intercepted by the selected area aperture is used for the boundary condition. It is known that a spherical aberration of an objective lens generally causes area-selection-errors in the SAD. To remove the errors, we use a Cs-corrector for imaging system in the present study, which is referred as the selected area nano diffraction (SAND) [2]. In this study, we have reconstructed an exit wave field from a SAND pattern obtained from a silicon {011} thin film. The dumbbell structure with a separation of 0.136 nm is resolved clearly in the resultant image[3]. It is concluded that the combination of the SAND and the diffractive imaging is effective in obtaining images with atomic resolution.

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Universal tree of species evolution

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