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

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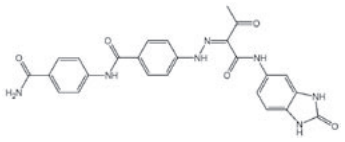
Pigment Yellow 181 is an industrially important reddish yellow pigment. The pigment usually crystallizes in thin needles. With a special additive a plate-like morphology can be obtained. [1] The platelets are arranged into a porous microsphere structure. Molecular modelling was used to study the influence 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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Keywords: diarylethene, theoretical crystal calculations, elastic properties

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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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Keywords: image reconstruction, electron diffraction techniques, selected area electron diffraction

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Universal tree of species evolution

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Protein sequences derived from the over 4 million genes have the potential to produce an evolutionary tree that unequivocally and accurately traces the divergent course of evolution of all species. Evolutionary trees rely upon identifying an essential protein present in all species. The short chain oxidoreductase (SCOR) family is a family of such proteins. One subgroup of the SCOR family has 11,000 members in the gene bank including from 5 to 50 members in all species. There is not one fully conserved residue in the family and the enzymes vary in length from 240 to 350 residues. By combining structural information in the Protein Databank with sequence data we are able to align over 98% of all family members. From this alignment we can determine the mechanism of cofactor binding, probable function, preferred aggregation state and subtle variants in mechanism of action of each. We can accurately catalog 30% of the sequences as to their specific substrates and characterize the topology of highly specific substrate binding pockets for an additional 50% of the structures as they cluster in substrate sequence space. Analysis of the substrate specific subgroups permits the identification of residues responsible for protein/protein interactions. Analysis of insertions and deletions in the loops connecting the beta-sheets and alpha helices of the Rossmann fold reveals correlations between indels in the loops and speciation. By examining and sorting all 11,000 SCOR sequences, as Gregor Mendel sorted peas and Barbara McClintock sorted corn kernels, it is possible to determine the exact details of 3 billion years of divergent evolution of species, sequence, three-dimensional-fold, and substrate specificity.

Keywords: evolution, substrate, rossmann fold

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Structure of dengue virus - Implications for flaviviral assembly and opportunities for drug design

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Epidemic flaviviral diseases are widespread in tropical regions and are caused by infections due to viruses such as Dengue, Yellow Fever, Japanese Encephalitis and West Nile viruses. Various therapeutic targets have been identified from structural studies, including structural proteins such as envelope (E), membrane (M) and capsid (C) proteins, and non-structural proteins, e.g. viral protease, helicase, RNA polymerase and methyl transferase. Currently there is no commercial vaccine or antiviral drugs for dengue infection, many ongoing research programs are focused on developing potential drugs against dengue virus. Dengue envelope protein involves protein-cell membrane interaction which leads to viral cell entry. We have performed phylogenetic analysis of envelope protein of dengue viruses from Southeast Asia from 1990 - 2007, built the homology model of envelope protein of several emerging Singapore strains, and compared with available crystal structures of dengue envelope protein. A putative ligand-binding pocket was identified, its conformational change is crucial to dengue virus membrane fusion. Further docking studies on envelope protein inhibitors provide insights into the role of binding pocket and facilitate the design of novel potent inhibitors against evolving dengue diseases.

Keywords: homology modeling, structure-based drug design, virus structures

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Photochemical neutral radical induced nucleation of proteins

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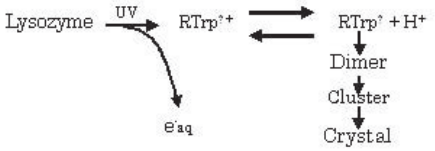
The crystallization is one of the bottlenecks for the protein X-ray crystallography. We reported that the number of crystals of hen egg-white lysozyme increased in metastable solution by UV-light irradiation and this phenomenon depends on irradiation light wavelength.1 Neutral radicals of tryptophan residue ($RTrp^{\bullet}$) of lysozyme were observed by transient absorption measurements. The photochemical dimerization of lysozyme was observed by SDS-PAGE for this solution. These results suggested that the dimer plays role of the smallest cluster. Scheme 1 shows the mechanism of photochemically induced nucleation of lysozyme. The photochemical reaction of tryptophan residue of lysozyme is photo-ionization leading to the generation of radical cation ($RTrp^{\bullet+}$) and hydrated electron. The RTrp. of lysozyme formed by deprotonation of $RTrp^{\bullet+}$. We, here, demonstrate the results of crystallization experiments of lysozyme at some dimer quantities. The pKa value of $RTrp^{\bullet+}$ was estimated by transient absorption measurements under various pH conditions.



Scheme 1 The mechanism of photochemically induced nucleation of lysozyme.

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Keywords: protein crystallization development, photochemistry, photodimerization

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The three dimensional structure of red, yellow and green fluorescent proteins from Zoanthus

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The three-dimensional structures of the wild type red (zRFP574), yellow (zYFP538) and green (zGFP506) fluorescent proteins (FP), from button polyp Zoanthus have been determined at 1.51 Å, 1.8 Å and 2.2 Å respectively and crystal structures of the zGFP506 mutant variant (zGFP506_N66D) with replacement of the chromophore first residue, Asn66Asp, in transition ‘green’ and matured ‘red’ states have been determined at 2.4 Å and 2.2 Å respectively. The novel posttranslational modification of the chromophore-forming sequence -Asp66-Tyr67-Gly68- in zRFP574 expands the protein maturation beyond the green-emitting form and results in decarboxylation of the Asp66 side chain. It was suggested that the electrostatic conflict between closely spaced, negatively charged side chains of the chromophore Asp66 and the proximal catalytic Glu221 is most likely the trigger of the reactions chain resulting in the observed