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Keywords: SAXS, structures of metalloorganic complexes, nanotechnology

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Drastic modulation of solid-state luminescence derived from molecular arrangement of organic salts

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Polycyclic p-conjugated molecules, such as anthracene and pyrene, are employed in many systems owing to their electro- and photophysical properties. Their properties in solid state depend not only on the molecular structure but on the molecular arrangements. As for the photoluminescent properties, there are several reports on the relationships with molecular arrangements. However, the relationships have not been elucidated exactly and therefore further study is necessary for the application to the development of sophisticated organic devices. Here, we present drastic modulation of luminescent color triggered by change of the anthracene arrangement of ammonium anthracene-1,8-disulfonate. The organic salts gave seven kinds of anthracene arrangements depending on the amine of the salts. Alkyl chain of n-butylamine surround anthracene moieties, resulting in blue luminescence attributed to monomer emission. Whereas, s-butylamine afforded formation of dimer pairs and contact of the pairs, resulting in orange luminescence attributed to excimer emission. Up to 150 nm of red shift depending on anthracene arrangements was achieved.

Keywords: organic crystals, luminescence, properties and structure relationships

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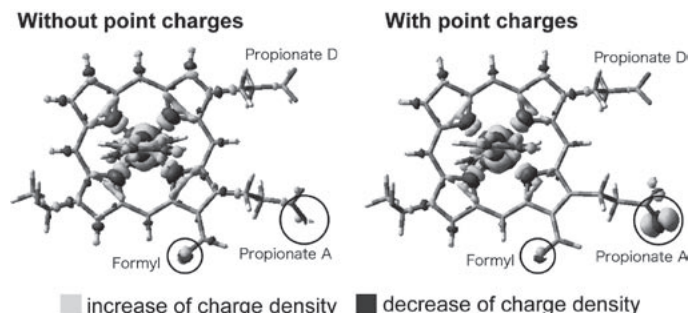
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Electronic structures of heme a of cytochrome c oxidase in the redox states

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The electronic structures of heme a of cytochrome c oxidase in the redox states have been investigated by using the UB3LYP method. Heme a is involved in not only electron transfer process but also in proton translocation process, which has recently been proposed by using X-ray structures at high resolution. We found that the most stable electronic configurations of the d electrons of the Fe ion were determined by the orbital interactions with the p orbitals of the porphyrin ring and the His residues. The redox reaction of the Fe ion influences the charge density on the peripheral parts of heme a, such as formyl and propionate groups, through the pi conjugation of the porphyrin ring and the orbital interaction with the sigma* orbital

of the C-C bond of the propionate group. The point charge model implies that electric field generated by surrounding protein enhances the charge transfer from Fe ion to the propionate group. The atomic charge differences of these groups are insensitive to distortion of the porphyrin ring, implying that heme a could be a "flexible electron mediator". The present results show why heme is ubiquitous in the biological systems.



Keywords: heme proteins, density functional theory, cytochrome oxidase

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Functional annotation by sequence-weighted structural alignments

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A method to functionally annotate "hypothetical" proteins, based on a novel structural alignment scoring function, is introduced. In the proposed method, position specific scoring matrices are used to weight structurally aligned residue pairs, highlighting evolutionarily conserved motifs. The functional form of the score is first optimized for discriminating domains belonging to the same Pfam family from domains belonging to different families but the same CATH or SCOP superfamily. The alignment method is next applied to the task of functionally annotating 230 query proteins released to the public as part of the Protein 3000 structural genomics project in Japan. Of these queries, 49 were found to match distantly related templates (seq ID < 30%). Within this group, the template predicted by our method to be the closest functional relative was often not the most structurally similar. Nevertheless, in a number of cases, the scoring function was able to identify key residues in the query that are likely to be involved in biochemical function. Several such nontrivial cases are discussed in detail.

Keywords: structural genomics, position-specific scoring matrix, maximum substitution probability

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Formation of ϵ -martensite (ϵ -Fe) in stainless steels

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ϵ -martensite (ϵ -Fe) [1] is one of four forms of crystalline iron besides