Construction and Photodynamics of a Supramolecule Composed of Saddle-Distorted Zinc-Phthalocyanine Complexes and a Diprotonated Porphyrin with Saddle Distortion

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Angewandte Chemie International Edition, **47**, 6712-6716 (2008)

Porphyrins and phthalocyanines have so far been utilized separately as important components to construct efficient light-energy conversion systems, undergoing efficient photoinduced electron transfer. We have demonstrated saddle-distorted dodecaphenylporphyrin (H_2DPP) can be easily protonated to give a stable dication, H_4DPP^{2+}, which can act as an electron acceptor. On the other hand, saddle-distorted octaphenylphthalocyanine (H_2OPPc) has been reported to form metal complexes, showing lower oxidation potentials compared to those of metal complexes having conventional planar phthalocyanines.

Now we have succeeded in the synthesis and the first crystal structure determination of a discrete supramolecular conglomerate composed of both phthalocyanine and porphyrin, i.e., Zn(OPPc) and H_4DPP^{2+}. Those components are linked by 4-pyridine carboxylate (4-$PyCOO^-$) as an axial ligand of the Zn(OPPc) units and a hydrogen-bonded counter anion of H_4DPP^{2+} (Fig. 1). This conglomerate was revealed to hold its architecture in $CDCl_3$ as evidenced by ^1H diffusion ordered spectroscopy (^1H DOSY). Femtosecond laser flash photolysis of the supramolecule in benzonitrile (PhCN) demonstrated that *intra-supramolecular* electron transfer occurred from the Zn(OPPc) unit to the H_4DPP^{2+} moiety to generate an electron-transfer state with the lifetime of 667 ps (Fig. 2). This is the first observation of an electron transfer of a supramolecular conglomerate including both porphyrin and phthalocyanine. Our strategy can pave a way to construction of novel supramolecular assemblies consisting of porphyrins and phthalocyanines to develop photofunctional materials that can utilize a wide range of visible light effectively.

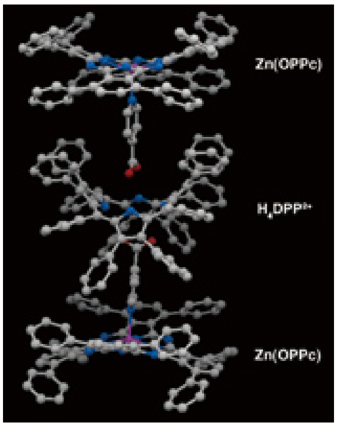

Fig. 1 The crystal structure of the supramolecule. Dark gray carbon, blue nitrogen, red oxygen, pink zinc. Hydrogen atoms are omitted for clarity.

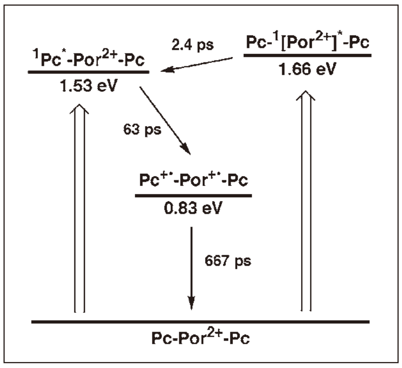

Fig. 2 The energy diagram of photodynamics of the supramolecule in PhCN. Por^{2+} and Pc represent the H_4DPP^{2+} and Zn(OPPc) units, respectively.

A Decompression Pipeline for Accelerating Out-of-Core Volume Rendering of Time-Varying Data

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Computers & Graphics, **32**, 350-362 (2008)

Volume rendering of time-varying data is to produce animation sequences that show how the three-dimensional structure evolves over time. This technique is useful to understand complex phenomena. One technical problem in time-varying volume visualization is the large amount of data. For example, a time-varying volume of 512x512x512 voxels with a hundred of time steps requires 12.5 GB of memory if each voxel has 1-byte data.

To deal with this problem, we have developed a decompression pipeline capable of accelerating out-of-core volume rendering of time-varying scalar data. Our pipeline is based on a two-stage compression method that cooperatively uses the CPU and the graphics processing unit (GPU) to transfer compressed data entirely from the storage device and the video memory (Fig. 1). The method combines two different compression algorithms, each designed for the CPU and the GPU, respectively.

Our pipelined renderer runs on a quad-core PC and achieves a video rate of 41 frames per second (fps) in average for 258x258x208 voxel data with 150 time steps (Fig. 2). It also demonstrates an almost interactive rate of 8 fps for 512x512x295 voxel data with 411 time steps.

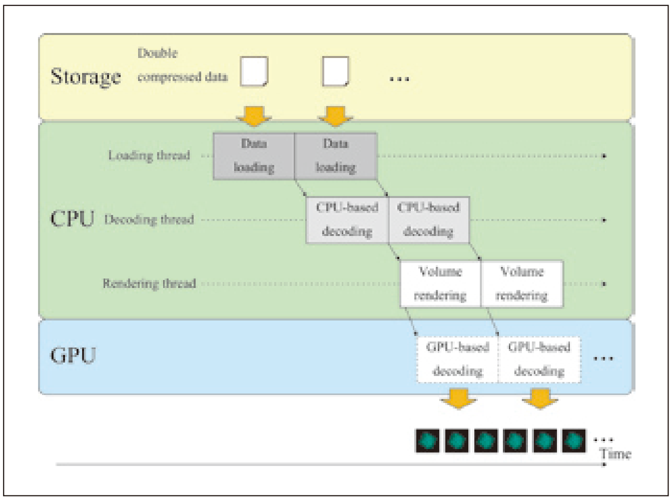

Fig. 1 Decompression pipeline implemented using multiple threads running on a multi-core CPU. The pipeline consists of three stages, each responsible for data loading, CPU-based decompression, and rendering with GPU-based decompression.

(a)

(b)

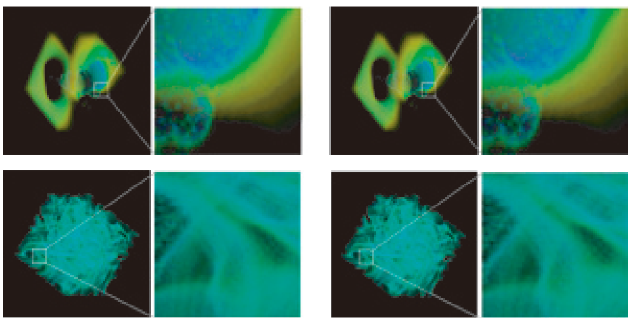

Fig. 2 Comparison of rendering results using (a) turbulent jet data and (b) turbulent vortex data. The left-hand side is the result from raw data while the right-hand side is that from compressed data.

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