Computational Materials Design: Porphyrins as Building Blocks of Designer Materials

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We entered the 21st Century witnessing several remarkable progress in Science and Technology. Novel materials and devices that were once considered the stuffs of *science fiction* are, one after the other, becoming a reality. It would not be an exaggeration to say that we are coming to the ***Age of Designer Materials***.

Complex materials are designed to have desired properties, with both basic and technological applications. Some present day examples include artificially patterned structures, forever smaller integrated circuits, magnetic storage devices, composite materials, polymer blends, doped transition metal oxides, self-assembling nano-structures, molecular electronics, etc.

The unifying themes that have emerged in the last several years are:

i. *quantum* size effects (in association with new phenomena in the nanoscale);
ii. *complexity* (in association with new phenomena emerging from the collective interaction of simple structures);
iii. *functionality* (in association with the new properties emerging as a response to changes in the environment).

A ***Designer Material*** has to do something. It has to be ***Functional***. It makes no sense to fabricate a *nanoscale* material that is *complex* and yet *does nothing* when its environment changes. We want a material that has many varied and competing ground states so that an external stimulus (heat, pressure, electric field, magnetic field, etc.) can be used to *switch* its properties.

At the same time, we can ask such questions as:

- *Can we achieve an understanding of collective phenomena to create materials with novel, useful properties?*
- *Can we design materials having predictable, and yet often unusual properties?*
- *Can we design and construct multicomponent molecular devices and machines?*
- *Can we harness, control , or mimic the exquisite complexity of nature to create new materials that repair themselves, respond to their environment, and perhaps even evolve?*
- *Can we develop the characterization tools and the theory to help us probe and exploit this world of complexity?*

To address the questions raised above, and to test the concepts and principles developed for realizing *designer materials*, we use ***Surfaces*** as our *playground/testing ground*. Allowing us access to the appropriate reduced dimensionality and means to manipulate the degree of complexity, and emergence of function.

At the symposium, time permitting, we will discuss about the current state-of-the-art in Materials Design, esp., efforts being made to employ Computational Materials Design (CMD) techniques (cf., e.g., [1-3]), together with the associated (Surface) Reaction Design (CRD) techniques (cf., e.g., [4]). For the examples, we pay particular attention to what Nature has given us as benchmark systems, i.e., bio-inspired materials design (esp., porphyrins-based materials), and also the role and advantage of inducing spin polarization, and controlling the dynamics of the reaction partners. We focus on the designer materials for Fuel Cells, (Nano)Spintronics [5], and other applications [1–6].

References:

[1] H. Kasai, H. Akai, H. Yoshida, Computational Materials Design from Basics to Actual Applications, Osaka University Press (2005) (in Japanese).
[2] H. Kasai, M. Tsuda, Computational Materials Design, Case Study I: Intelligent/Directed Materials Design for Polymer Electrolyte Fuel Cells and Hydrogen Storage Applications, Osaka University Press (2008) (in Japanese).
[3] H. Kasai, H. Kishi, Computational Materials Design, Case Study II: Intelligent/Directed Materials Design for Resistance Random Access Memory, Osaka University Press (2012) (in Japanese).
[4] H. Kasai, H. Kasai, W.A. Diño, R. Muhida, Prog. Surf. Sci. 72 (2003) 53.
[5] Spintronics (a new-coined word meaning "spin transport electronics"), also known as magnetoelectronics, is an emerging technology that exploits both the intrinsic spin of the electron and its associated magnetic moment, in addition to its fundamental electronic charge, in solid-state devices, in the *nano*-scale dimensions.
[6] For further specific references, *cf., e.g., www.dyn.ap.eng.osaka-u.ac.jp/pub.html*.