新学術領域「コンピューティクスによる物質デザイン：複合相関と非平衡ダイナミクス」
計画研究／公募研究「ｘｘｘｘ」

Computational Materials Design—from basics to applications

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The increasing demand for more advanced technology, coupled with the astonishing development of nanotechnology in the 21st century, necessitates the more advanced techniques in the elucidation of material function formation mechanisms and realization of new generation functional materials. Complex materials such as artificially patterned structures, nanosized integrated circuits, magnetic storage devices, composite materials, polymer blends, doped transition metal oxides, self-assembling nanostructures, molecular electronics, among others, are engineered and designed to have the desired properties for basic and technological applications. In the design of functional materials, relevant questions arise:

-Can we achieve an understanding of collective phenomena to create materials with novel and useful properties?

-Can we design materials which have predictable, and yet often unusual properties?

-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?

With the advent of advanced computational facilities and techniques, Computational Materials Design (CMD®) [1] is now a reality. Here, the fundamental properties of materials are accurately calculated through first-principles (ab-initio) calculations; that is, the properties of materials are calculated accurately from fundamental equations of quantum theory without empirical parameters. Its impact on industrial research and development has become very significant in the past years and is expected to grow in the coming years with the explosion of the number of granted patents purely based on CMD.

In the conference, the current state-of-the-art facilities in Materials Design, esp., efforts being made to employ CMD techniques (cf., e.g. [1,2]), together with the associated (Surface) Reaction Design (CRD) techniques [3] will be discussed; highlighting benchmark systems such as bio-inspired materials design, role of inducing spin polarization, and controlling the dynamics of reaction partners, with special attention to Fuel Cell and (Nano) Spintronics applications [1-5].

References:

[1] H. Kasai, H. Akai and Y. Yoshida, Computational Materials Design from Basics to Actual Applications, Osaka University Press (2005) (in Japanese).

[2] H. Kasai and M. Tsuda, Intelligent/Directed Materials Design for Polymer Electrolyte Fuel Cells and Hydrogen Storage Applications, Osaka University Press (2008) (in Japanese).

[3] H. Kasai, W.A. Dino, R. Muhida, Prog. Surf. Sci. **72** (2003) 53.

[4] For further specific references, cf., e.g., www.dyn.ap.eng.osaka-u.ac.jp/pub.html.

[5] Spintronics (a newly 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. (US Patent No. 7,432,572, B2).