Activity Reports of Materials Design through Computics: Complex Correlation and Non-equilibrium Dynamics

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Scientific Research on Innovative Areas by MEXT during July 2010 and March 2015

PREFACE

This booklet is a report of a research project ``Materials Design through Computics: Complex Correlation and Non-equilibrium Dynamics" conducted as a ``Scientific Research on Innovative Areas" supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. The project started in July of 2010 and successfully ended in March of 2015. The research project was conducted by 45 research groups including 135 researchers in total.

Computational approach to science was started around 1960s. An approximation called Hartree-Fock approximation in describing the electron-electron interaction was developed and applied to a variety of molecules in 60s with the aid of computers.[1] Density-functional theory (DFT) innovated by Walter Kohn, Pierre Hohenberg and Lu Sham in 1964 had been developed in 60s and 70s and provided a firm theoretical framework and actual prescriptions to calculate electron states of not only molecules but also condensed matters.[2] Today, computational science is recognized as the third approach which complements the previous two approaches, experimental and theoretical, and allows us to access new aspects of phenomena in nature.

One of the typical stances of people in the field of computational science has been solving the basic equations with the aid of computers. Computers themselves have been black boxes for scientists in physics and chemistry. Collaboration between physical/chemical science and computer science or information technology has been very rare.

Current dramatic change in computer architecture is awakening scientists with this happy and old stance. The performance of a single CPU or a compute core is already saturated, corresponding to the limitation of Moore's scaling law on the device integration. Then the only way to make a supercomputer is gathering a huge number of compute cores and nodes and connecting them with high speed networks. The K computer at Kobe, Japan, for instance, which shows the peak performance of 10.62 PetaFLOPS is composed of 640 thousands compute cores connected by the 6-dimensional Tofu (Torus Fusion) networks. In the coming supercomputers, in addition to such many-core massively parallel architecture, some hardware accelerators should be introduced.[3] Owing to this complexity in the current and next computer architecture, it is almost impossible to exploit potential power of the supercomputers, unless we tune our application codes progressively. The tuning in this context means not only improvements of the existing application codes but also

[1] The ``super"-computer in those days has the performance of only 1 MFLOPS (Mega FLoating-point Operations Per Second) [CDC 6600, (1964)], being much slower than the current personal computers.
[2] A systematic calculations for the structural characteristics and energy bands for simple metals are performed and documented in 1978 (V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals*, Pergamon Press)
[3] Top500 supercomputing sites: http://www.top500.org/

developments of new algorithms suitable to the parallel architecture. The algorithms to solve the issues rely on mathematical methods. Hence the tuning includes innovation of new mathematical methodology to tackle most important scientific issues and then its implementation on the new computer architecture. This requires an effort to analyze basic equations describing phenomena in nature and innovate new algorithms. These efforts we call *compuics*. Mathematics has contributed a lot to progress in science since *Principia* by Isaac Newton. Computics in this century may be a new approach to clarify underlying principles in nature.

This project focuses complex correlation and non-equilibrium dynamics in phenomena in materials. Properties of materials are determined by competition of various physical and chemical interactions: Covalency, ionicity and metallicity are typical ingredients to determine properties of materials. Electron Correlation is also an important factor. In nano-materials and structures, nanoscale shape decisively affects the relevant wave-functions and then induces new properties hidden in bulk structures. We call this *complex correlation*. Femtosecond laser irradiation on materials, for instance, causes electron excitation and then ionic motions. It occasionally induces structural transformation. This is a new way of materials design by utilizing *non-equilibrium dynamics*.

In order to reveal complex correlation and non-equilibrium dynamics, developments of computational schemes along three axes are required. First, in the nanometer scale objects, quantum effects are important. On the other hand, 10-cube-nanometer objects are composed of 100 thousands atoms. Quantum mechanical electronic structure calculations for 100-thousands atoms are certainly unprecedented. This is a challenge along the space axis. Second, the electron excitation followed by the ionic motions is a multi-scale phenomena: Electron excitation takes place in femtosecond timescale and ionic motions are in picoseconds; structural transformation requires nano-, micro, or even mili-seconds. We are challenged along the time axis. Thirdly, materials are composed of many electrons and nuclei. In describing their electronic properties, materials are regarded as interacting electron systems. Accurate calculations based on quantum mechanical many-body theory are indispensable. This is a challenge along the accuracy axis. In our projects, many efforts have been done on these lines.

This report consists of three parts. In Part I, activities in ``Architecture and Algorithms of High Performance Computing" are reported. They are mainly in the field of computer science and/or applied mathematics. But the collaborations between this field and the field of computational materials physics are also reported. Principal investigators in this Part are Mary Inaba (University of Tokyo), Daisuke Takahashi (University of Tsukuba) and S.-L. Zhang (Nagoya University). Activities of other two research groups performed during 2013-2014 are also reported in Part I.

Part II is devoted to the activities in ``New Development in Density-Functional Theory". Density-

functional theory (DFT) has been contributing tremendously to reveal materials properties in these decades. The exchange-correlation functional which describes many-body effects is still improved and widens a set of the target materials which are described by DFT. Efforts along the space axis and time axis are also documented in Part II. Principal investigators in this Part are Atsushi Oshiyama (University of Tokyo), Shinji Tsuneyuki (University of Tokyo), Satoshi Watanabe (University of Tokyo), Hiroshi Nakanishi (Osaka University) and Takahisa Yamato (Nagoya University). Activities of other nine research groups including experimental works performed during 2013-2014 are also reported in Part II.

In Part III, activities in `` Beyond Density-Functional Theory" are reported. Current DFT has certainly limitation. In particular, materials with strong electron correlation are difficult to be treated by the current DFT. Theory and computational schemes which are beyond DFT are certainly important. In our project, several efforts based on the perturbation theory, a new down-folding approach and so forth have been done. Principal investigators in this Part are Masatoshi Imada (University of Tokyo), Yasutami Takada (University of Tokyo) and Kazunori Sato (Osaka University). Activities of other seven research groups including experimental works performed during 2013-2014 are also reported in Part III.

Research activities achieved by other ten research groups during the period of 2011 – 2012 are not included in this booklet due to the limitation of the pages. The activities are accessible on the computics web page, http://computics-material.jp/index-e.html. The researchers in the ten projects include I. Hamada (NIMS), M. Hase (University of Tsukuba), H. Hirayama (Tokyo Institute of Technology), H. Ono (Kyushu University), F. Shimojo (Kumamoto University), M. Kitajima (National Defense Academy), M. Saito (Kanazawa University), H. Tanaka (Osaka University), Y. K. Zhou (Osaka University) and T. Kotani (Tottori University).

The online version of this report is available thorough http://computics-material.jp/index-e.html. I wish this booklet contributes to the progress in a new growing field, *computics*.

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Complex Correlation and Non-equilibrium Dynamics

CONTENTS