Title of Project : Materials Design through Computics: Complex Correlation and Non-Equilibrium Dynamics

Term of Project : FY2010-2014

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【Purpose of the Research Project】

A new challenge is facing condensed-matter science today. It is to propose a new paradigm for manufacturing based on quantum theory. Progress in fabrication technique almost allows us to place each atom on a desired place to make new structures and materials. The issue is that which elements and what struc- tures we should fabricate to obtain new func- tions. Computational science based on quantum theory is able to make essential contributions to this challenging task of materials design since it stands on deep scientific truth.

The purpose of the present project is twofold: First, we aim to establish a new science field named computics, which is a fusion of computationnal and computer sciences, by developing novel approaches in rapidly changing circumstances of the computer architecture. Second, by innovatively developing the quantum theoretical methodology and collaborating closely with experimental research, we aim to clarify and predict complex correlation and non-equilibrium dynamics which are unresolved issues in materials design. We hereby aim to change the paradigm for manufacturing from the empirical to the deductive.

【Content of the Research Project】

The 3 research domains, A01 computer architecture and high-performance algorithm, A02 development of the density functional theory (DFT), and A03 beyond the DFT for correlated systems, are organized, and the 11 research groups has joined and additional groups will join the project. In the domain A01, we focus on the high performance computing (HPC) in the next-generation architecture and a new algorithm for large-scale linear equations, and the actual HPC is realized for scientific tasks raised from A02 and A03 research domains. In the domain A02, the DFT and the time-dependent DFT are developed progressively and combined with several methodologies exploring dynamics in materials. In the domain A03, new theoretical schemes are developed beyond DFT to pursue underlying physics in strongly-correlated materials. Clarifying and predicting complex correlation and non-equilibrium dynamics in materials syntheses, electron, heat and atom transports, bio-reactions, correlated materials, and superconducting phases are the research targets.

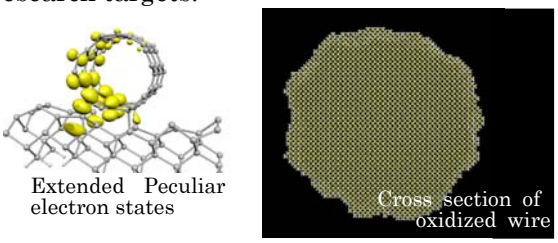

Figure: Calculations have revealed atomic and electronic structures of carbon nanotubes on the stepped Si surface (left), and the electron density of the Si nanowire (right).

【Expected Research Achievements】

Advanced scientific calculations based on quantum theory which are unprecedented in scale and quality will be feasible by utilizing advantages of the future computer architecture, and then the complex correlation and the non-equilibrium dynamics in wide range of materials are expected to be clarified. In collaboration with experimental research, a new deductive methodology for the materials design will be established. It is expected that new materials and structures which can be boosters in the future technology are proposed.

From science viewpoints, by expanding frontiers of quantum science calculations, the fundamental methodology in basic science will be deepened, and hence new quantum phases could be discovered through computics.

【Key Words】

Computics: An interdisciplinary science field in which computational and computer sciences are fused to develop new computational methodologies in natural science.

【Homepage Address】

http://computics-matreial.jp/