【Grant-in-Aid for Scientific Research (S)】

Science and Engineering (Mathematical and Physical Sciences)

Title of Project : Materials Design and Exploration of Functions for Strongly Correlated Materials – Challenges to Non-Equilibrium and Non-Periodic Systems

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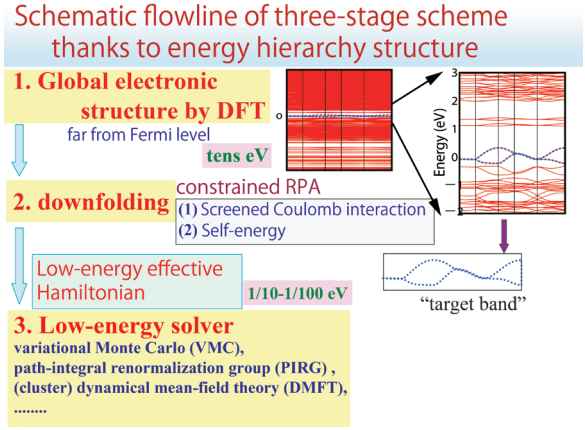
Research Project Number : 16H06345 Researcher Number : 70143542
Research Area : Physical Sciences
Keyword : Strongly Correlated Materials, Non-equilibrium Systems, Interfaces, First-Principles

【Purpose and Background of the Research】

Electron correlations have been one of the central fields to cultivate novel concepts in basic science, which have novel functions and potential applications as well. However, strongly correlated materials were faced with difficulties in theoretical and computational tools for their studies. Recently this challenge has been greatly explored and a powerful method called multi-scale ab initio scheme for correlated electrons (MACE) (bottom figure) has been pursued and successfully applied.

In this project, we extend this scheme to 1. non-equilibrium phenomena and 2. non-periodic systems such as surface, interface and quasicrystals and pioneer frontiers of strong correlation physics. Above all, a. non-equilibrium high-temperature superconductivity, b. principles for efficient solar cells, c. theories to analyze time-resolved experimental probes, d. high-temperature superconductivity on interfaces and thin films, e. topological mobile and tunable interfaces such as magnetic domain walls, f. anomalous thermal and electronic conduction of quasicrystals, and g. magnetism at grain boundaries of permanent magnets are suitable subjects to be pursued by developing our methods. Mechanisms and functions of novel phenomena in charge-spin-lattice coupled systems will be studied with emphasis on transition metal compounds based on MACE towards the goal of materials design of strongly correlated electron materials.



【Research Methods】

[Methodologies] (1) We implement methods for non-equilibrium states and excitations by extending variational Monte Carlo (VMC), and dynamical mean- field (DMFT) methods as well as many-body perturbation methods including the vertex corrections. (2) We improve methods to treat non-periodic systems (surfaces, interfaces and quasi-crystals) by taking account of structural relaxations. (3) We extend VMC and DMFT for electron-phonon interaction, spin-orbit interaction and multi-orbital systems. Emergent excitations as well conventional collective excitations are examined. Open source codes will be released after developing codes for general use.

[Application to materials design] We clarify mechanisms of non-equilibrium high-temperature superconductivity, general principles for materials design of efficient solar cell design. After taking account of lattice relaxation and electron-phonon interaction, designing high- temperature superconductivity at interfaces and thin films and functional topological interfaces are explored.

【Expected Research Achievements and Scientific Significance】

Basic science and materials design of strongly correlated systems will be developed based on first principles methods.

【Publications Relevant to the Project】

・F. Aryasetiawan, M.Imada *et al.*, "Frequency-Dependent Local Interactions and Low-Energy Effective Models from Electronic Structure Calculations" Phys. Rev. B **70** (2004) 195104.
・M. Imada and T. Miyake, "Electronic Structure Calculation by First Principles for Strongly Correlated Electron Systems" J. Phys. Soc. Jpn. **79** (2010) 112001.

【Term of Project】 FY2016-2020

【Budget Allocation】 85,400 Thousand Yen

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