

【Staff Members】

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【Research Activities】

Experimental study for GRID computing with supercomputers distributed in Japan based on the Nanotech-VPN on SuperSINET has been conducted by this research group using the original ab initio program TOMBO, which has been developed by our members during last 15 years. This project is known as a real large scale GRID computing and users are now expanding over the world. Applying the diffusion quantum Monte Carlo method, we have solved the long standing problem of Hund's multiplicity rule for atoms and molecules with high accuracy satisfying virial theorem (**Ref.5**).

Ab initio study on nanoclusters has been conducted in wide range of binary elements and obtained new magic number clusters and novel properties in these clusters (**Ref. 1, 3, and 4**)

Conducting polymers for nanotechnology have been studied by ab initio simulation and established a method to select the best candidate by genetic algorithm. Other important results of our research group are the standard experimental data analysis and design of bulk materials, where we have studied magnetic properties (**Ref.1**), piezoelectric materials, optical materials, etc. We have made a contribution to create and distribute materials fact database for nonequilibrium phase with the Center for Computational Materials Science, and obtained physical and chemical properties in binary amorphous alloys, artificial magnetic multilayers, high pressure data, etc.

1. Ultra-stable nanoparticles of CdSe revealed from mass spectrometry,
Kasuya A, Sivamohan R, Barnakov YA, Dmitruk IM, Nirasawa T, Romanyuk VR, Kumar V, Mamykin SV, Tohji K, Jeyadevan B, Shinoda K, Kudo T, Terasaki O, Liu Z, Belosludov RV, Sundararajan V, Kawazoe Y,
NATURE MATERIALS 3 (2): 99-102 FEB 2004
2. Antiferromagnetic coupling driven by bond length contraction near the $Ga_{1-x}Mn_xN$ film surface,
Wang Q, Sun Q, Jena P, Kawazoe Y,
PHYSICAL REVIEW LETTERS 93 (15): Art. No. 155501 OCT 8 2004
3. Origin of spontaneous electric dipoles in homonuclear niobium clusters,
Andersen KE, Kumar V, Kawazoe Y, Pickett WE,
PHYSICAL REVIEW LETTERS 93 (24): Art. No. 246105 DEC 10 2004
4. Smallest magic caged clusters of Si, Ge, Sn, and Pb by

encapsulation of transition metal atom,

Kumar V, Singh AK, Kawazoe Y, NANO LETTERS 4 (4): 677-681 APR 2004

5. Interpretation of Hund's multiplicity rule for the carbon atom,

Hongo K, Maezono R, Kawazoe Y, Yasuhara H, Towler MD, Needs RJ,

JOURNAL OF CHEMICAL PHYSICS 121 (15): 7144-7147 OCT 15 2004

【Plan】

One of the most important research projects in our group is to contribute to the fundamental problems in quantum physics by using large scale computer simulation. Recent rapid progresses in supercomputer technology and theoretical development of diffusion quantum Monte Carlo method have made it possible to solve exactly the many electron system without any approximations or models. Paper 5 is a successful example concerning the clarification of the reason of Hund's multiplicity rule, which has been explained based on the misunderstanding in most of the textbooks.

The present study includes the transition metals and the results will make more strong impact in the basic research. Another subject is a kind of new alchemy, which aims to design useful new materials based on large scale simulation without experimental parameters. We are focusing on materials for nanotechnology and working collaboratively with experimental groups and wide variety of various industries. Last plan is the long time database project, which was expected for this research group from the starting time. We have made an agreement with Springer-Verlag for the publication as of the Landolt-Boernstein series. Within this financial year we will publish the second volume of the nonequilibrium phase diagram, one of the most important experimental works from our Institute.