RICC Usage Report for Fiscal Year 2011

Project Title:

Computational Materials Science

Name :○John S. Tse, Toshiaki Iitaka
Affiliation :Computational Astrophysics Laboratory Advanced Science Institute,Wako Institute

1. **Background and purpose of the project**,

Pressure is a very sensitive probe for chemical bonding. Traditionally, much emphasis has been put on breaking new ground in achieving the highest pressure possible in the laboratory using either shock-wave or the diamond anvil techniques. Pressure up to 1 TPa has been achieved. Many new and exotic phenomena, such as quantum liquid phase, superconductivity etc. has been uncovered. More recently, a new direction in high pressure research has been in the very low pressure regime (i.e. between 1 -50 GPa). Studies on mixtures of close shell atoms, molecules, such as, SiH4 with H2, Xe with halogen molecules have revealed novel molecular complexes with unusual electronic properties can be formed. The motivation of this proposal is to continue our main research theme to develop a comprehensive scheme to rationalize the nature of chemical bonds between elements and molecules under these extreme conditions. Electronic structure calculations based on the density functional theory has been the main method to determine the electronic structure of these systems. A long term objective is to employ pressure to establish a structure-property correlation and to manipulate materials properties using external compression as the driving force, especially with low pressure.

2. Specific usage status of the system and calculation method

Most if not all calculations will be performed with the density functional pseudopotential plane wave electronic structure methods. In most cases, the generalized gradient approximation will be used. Highly efficient public domain codes VASP, SIESTA, WIEN2k and Quantum Espresso will be used. In addition, our own implementation (ASAP) of the genetic algorithm method will be used for structural search. Since most of the materials to be studied are close to insulator – metal transition, special care will be paid to the correct predict of the band gap energy. To this end, hybrid functionals, such as the HSE and perturbutative GW methods will be used to compute the electronic band structure. In addition, correlated treatment of the electronic spectra will be calculated from solving of the Bethe-Salpeter equation. Electron-phonon coupling will be calculated using the implementation in Quantum Espresso. For accurate evaluation of the electron-phonon coupling parameter, the new wannier function method will be employed.

3. Result and Conclusion

The calculations proposed are very time consuming. Unfortunately, due to the unexpected tragedy of the tsunami in March 2010, and the resulting restriction on the length of the computational time for each submitted job and the initial frequent shutdown of the computer to converse electricity, the project was inadvertently delayed. Moreover, the proponent was supposed to visit RIKEN as part of his

sabbatical leave in 2011. As a result, the proposed project no substantial results were obtained.

4. Schedule and prospect for the future

We wish to resume the project in fiscal 2012. The working schedule will be the same as proposed in the 2011 Usage Application.. As mentioned above, the major reason of the used time allocation is due to the uncertainty of the operation of the RICC computing cluster after the tsunami tragedy in March 2011. Now the computeing system is back to normal operation, we wish to continue the research in fiscal 2012.

Fiscal Year 2011 List of Publications Resulting from the Use of RICC

Jianjun Yang, John S. Tse and Toshiaki Iitaka, First Prcinples Study of Liquid gallium at ambient and high pressure, JOURNAL OF CHEMICAL PHYSICS 135, 044507 (2011).