THE UNIVERSITY OF TOKYO

RISS Research and Development of Innovative Simulation Software

RSS21 Revolutionary Simulation Software

First principles electronic structure calculation software

PHASE

PHASE
UVSOR
ASCOT

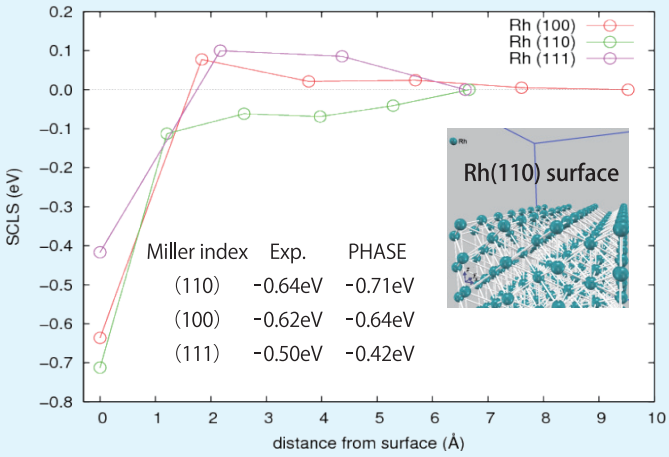
Implementable across a wide range of computing platforms!

From notebook PCs to PC clusters to supercomputers

First principle electronic state analyzing software based on the density functional theory with pseudo potentials and plane waves

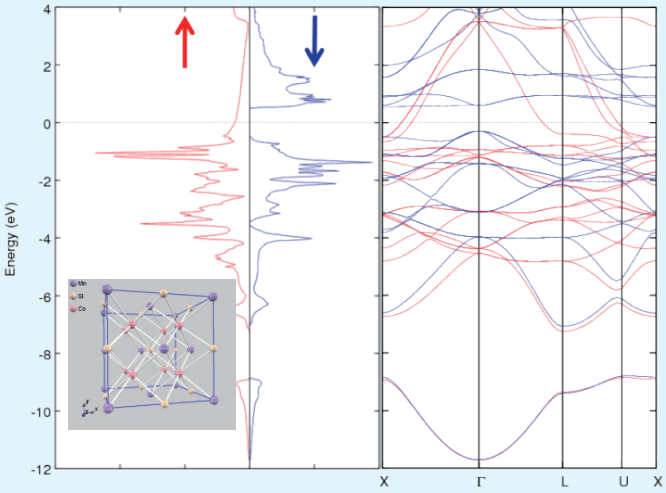
Feasibility Studies

XPS analysis for transition metals



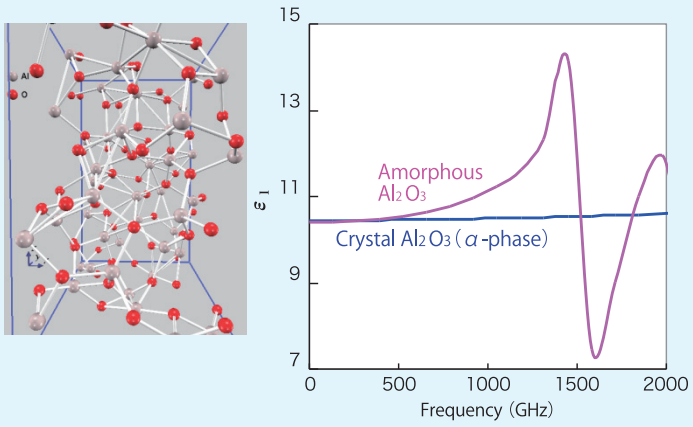
Core shift levels of Rh surfaces are calculated.
Obtained results are in good agreement with experimental data.

Band structures of a half-metal material



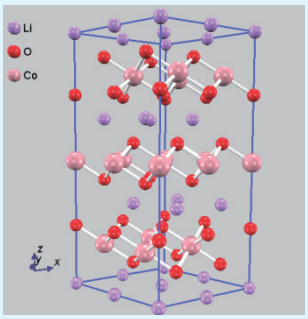
The band structure of a full Heusler alloy, Co_2MnSi. Metallic character evident for the up spin while insulator-like evident for the down spin.

THz range dielectric response analysis



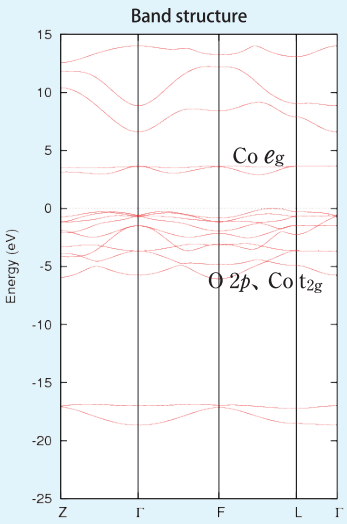
Dielectric function of amorphous and crystal alumina.
In this range the dielectric constants of these two systems are different.

Electrode potential analysis of Li ion battery material



Electrode potential

Exp.	PHASE
4.2V	4.5V

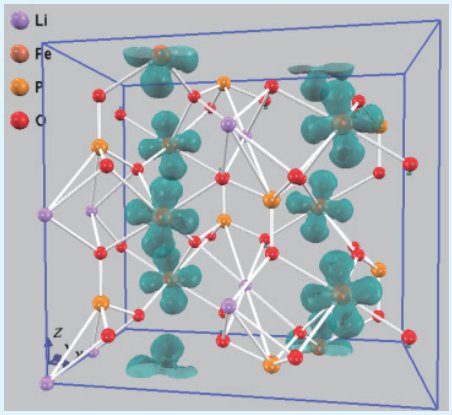


The electrode potentials are obtained from the energy difference between $LiCoO_2$ and CoO_2. Results have shown good agreement.

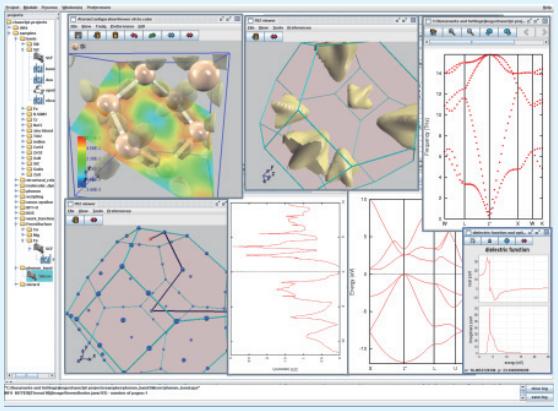
Feature works

- Applicable to various materials including metals, insulators, and semiconductors
- Designed for large scale parallel computing
- Implementable into various types of platforms (Windows PC, PC cluster, Earth Simulator…)
- Easy to use with provided GUI environment and supporting scripts

Electron densities around the Fermi level of $LiFePO_4$



Standard GUI environment PHASE-Viewer



Functions

Basic function	Total energy, Electron density, Structure optimization, Density of states, and Band structure
Exchange correlation potentials	LDA and GGA
Pseudo potentials	Troullier-Martins (TM) pseudo potential, Ultra-soft pseudo potential, and Projector Augmented Wave (PAW) potential
Molecular dynamics	Constant energy and Constant temperature
High accuracy electron state analysis	DFT+U, Hybrid functional, Van der Waals interaction, and TDDFT
Chemical reaction path analysis	NEB method, Blue Moon method, and meta dynamics method
Other functions	Vibration analysis, Stress tensor, Elastic constant, STM, XPS, AFM Dielectric function (electrons and lattice), Non-linear susceptibility, Piezoelectric constant, Wannier functions
Supporting software	GUI environment is provided to support the creation of input files and the drawing of output data Support scripts to help output analysis are also included

Platforms

Windows 2000, XP, Vista, 7 (Non-parallel binary distribution)

Linux work station and cluster (Fortran90 compiler)

Earth simulator

PHASE is supported by the project "Research and Development of Innovative Simulation Software (RISS)".

Liaison: Nanodevice simulation system R&D group (T. Ohno and T. Uda)
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