R&D field: Nano science

First-Principles Molecular Dynamics Simulation within the Plane-Wave Pseudopotential formalism

- Program name: PHASE
- Developer
  - Revolutionary Simulation Software Project
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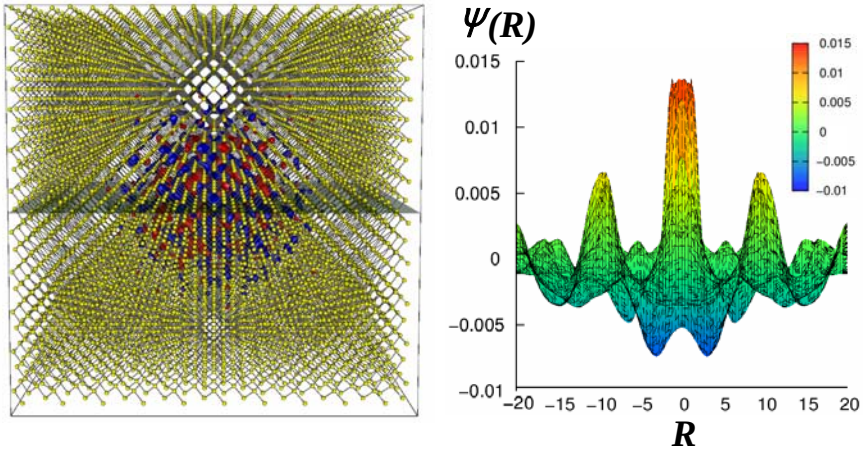
- Abstract
  - First-principles calculation of electronic states of matters.
  - Analysis of structures and properties of matters based on the quantum theory of the electron.
- Algorithm
  - Density functional theory.
  - Plane-wave basis set.
  - First-principles pseudopotential method.
  - Fortran90 and C.
  - Parallel computation with MPI.
- Current computation size
  - Analysis of As-donor levels in Si with 5832-atom super cells.
  - Sustained performance 13.6 TFLOPS (384 nodes of Earth Simulator).
  - Memory 3.1 TB and disk 0.2 TB.
- Future computation size in 2010
  - About 50,000 atoms.
  - Memory 50 TB and disk 2 TB.



A ground-state wavefunction of As donors in Si

- Expected results
  - Exploration of non-silicon devices beyond the scaling limits based on quantum-mechanical functional analysis of post-35nm-generation nano devices.
  - Realization of high-density magnetic storage (1Tbit/inch^2 or more) with first-principles analysis of vertical magnetic storage.
  - Development of gene-level therapy and clarification of mechanism of copy, damage, and repair of genes based on reaction analysis between enzymes and DNA/RNA.
- Reference
  - http://www.rss21.iis.u-tokyo.ac.jp/theme/multi/material/index.html