R&D field: Nano science

Ab-initio Molecular Dynamics Calculation in Real Space

- Program name: RSDFT
- Developer
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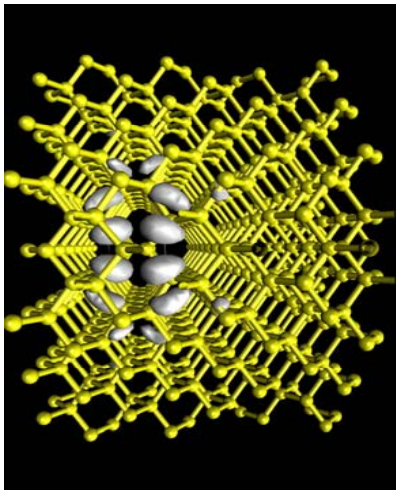
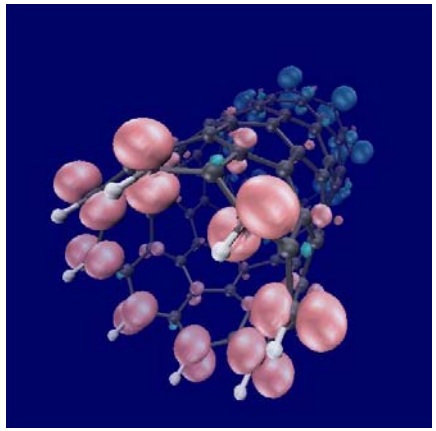
- Abstract
  - Quantum-mechanical nanoscale phenomena is investigated based on first-principle methods to estimate property and structure of nanomaterial having new functions.
  - The fundamental equations of the density functional theory is solved with the real-space finite-difference method to estimate structural stability, electron structure, and dynamics.
  - High effective performance of vector processors (more than 80 % on a CPU) and its feasibility for the next-generation supercomputer.
- Algorithm
  - The real-space high-order finite-difference and the Verlet methods.
  - Minimization of recursive energy with respect to the degrees of freedom of electron and ion.
  - Fortran90.
- Current computation size
  - Very accurate quantum mechanical calculation of 1,728 Si atoms. Sustained performance 235 GFlops (peak performance 358 GFlops) and memory 96 GB (64 nodes of PACS-CS of Tsukuba Univ.).
- Future computation size in 2010
  - Quantum mechanical calculation of 46,656 Si atoms (10 nm^3): memory 27 TB.



Electron cloud of levels induced by holes in Si



Spin magnetism in a carbon nanotube

- Expected results
  - Acceleration of material search with the post-scaling/Si technology based on the quantum-mechanical combinatorial method adopted in this research.
  - Finding of materials having new functions to advance the next-generation technology.
  - Establishment of guiding principles for nanotechnology fabrication based on quantum mechanics.
  - Creation of interdisciplinary research subjects based on nano- and bio-materials with a common quantum-mechanical method.
- Reference
  - http://www.px.tsukuba.ac.jp/home/tcm/oshiyama/HP/index_j.html