Computational Science Center

• Brief History of CSC
  - Nov. 2003: 1024 cpu Linux cluster system (2.85 Tflops) set-up
  - 2005 and 2006: The best research group awards in KIST
  - Jan. 2007: Computational Science Center Launched.

• Highlight Publications (2007~2008)
  - Cu doped GaN: Nano Letters, 7, 3366 (IF=9.960)
  - Me-C bonds: Carbon, 46, 185 (IF=4.260)
  - Protein structure calculation: J. Comp. Chem, 28, 2552 (IF=4.893)

• Nano and Bio Technology
  - (sub)atomic scale understandings of structure, kinetics and properties

• Organizational Chart

- Head of CSC: Kwang-Ryeol Lee

- HPC & Bio Simulation
  - Kye-Ho Lee

- Interface & Surface
  - Min-Mook Oh
  - Hwanwon Chung

- Nano-materials Simulation
  - Jung-Mee Choi
  - Seung-Chul Lee

- Myoung-Woon Moon

• Simulation Scope

- Computational science can reduce time and cost for R&D increase research efficiency

- Traditional → Computation → Experiment

- Researchers & Developers
  - Virtual Reality
  - User I/F
  - Multiscale Simul. Codes
  - Massive Computation

- Potential Development
  - Computation
  - Theory
  - Experiment

- Computational science can reduce time and cost for R&D increase research efficiency

- Optimization algorithm
  - Genetic algorithm

- Ab-Inito Calculation

- Molecular Dynamics

- Synth. & Appl. of Nanostructure Surface

- Fundamental understanding of surface nanostructures
  - Bio-implant Application of Nanostructure
  - Fuel cell nano-fiber: Energy
  - Synth. & Appl. of Nanostructure Surface

- HPC & Bio Application

- Visualization & Analysis

- Molecular Dynamics

- Ab-Inito Calculation

- Visualizations & Analysis

- Structure of Si (001) vicinal surface

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- CNT buckling by sonication

- Stable Phase of Ni Nanocluster

- Asymmetric surface intermixing during thin-film growth in the Co–Al system

- Strain effects on Ge thin films

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High Performance Computing & Bio Simulation

- **Hardware/Software Infrastructure**
  - KIST Linux Cluster 1,024 CPUs

- **Bio Simulation**
  - All-Atom De novo Protein Folding with a Scalable Evolutionary Algorithm

- **Visualization**
  - 3-D Stereo Graphic System

- **Simulation Softwares**
  - LAMMPS
  - EAM/MEAM
  - SiON FF
  - Brenner Polymers FF
  - Tersoff
  - SIESTA
  - TB Calculation
  - Kinetic MC
  - Ab initio MD & MC

- **Optimization & Algorithms**
  - Optimization
    - Genetic Algorithm, Simulated Annealing, etc.
  - Optimization & Algorithms
  - Optimization

- **PLSi Project**
  - Partnership & Leadership for nationwide Supercomputing Infrastructure

- **KIST Linux Cluster for ab-initio Calculation**
  - OS: CentOS 5.2
  - CPU type: Quad-core Intel Xeon E5450, 3.0GHz
  - Number of Nodes: 16
  - Number of Cores per node: 8
  - Memory per node: 32 GB
  - Interconnection Network: Myrinet 10G NIC & Switch
  - File Server: 25 TB (GFS, GPFS client)

- **TozongDock: Application of Stochastic Optimization to Protein-Ligand Docking**

- **Visualization**
  - Crystal eye glasses X 5
  - Stereo Projector

- **Optimization**
  - Genetic Algorithm, Simulated Annealing, etc.
**First Principles Calculation of Materials**

- **Softwares for Ab-Inito Simulations**
  - VASP: Plane-wave pseudopotential
  - WIEN2k: Full potential LAPW
  - CRYSTAL06: Atomic orbital
  - ABINIT, CPMD, SIESTA

- **Utilities**
  - Nudged Elastic Band
  - ATAT

- **Search for New Functional Materials**
  - Diluted Magnetic Semiconductors: Cu doped GaN
    - Zinc Blende GaN
    - Magnetization Density
    - Density of States

- **Search for New Functional Materials:** Monte Carlo + Ab-Initio
  - Si$_{50}$Ge$_{50}$ 1-Dimensional Nanowire

- **Understanding Bond Nature**
  - Metal Incorporated Carbon

- **Strain Effects - Nanowire**
  - Dopant Configuration in GaN-nanowire

- **Strain Effects – Thin Film**
  - Ge on Biaxial Compressive Strain

**Schrödinger’s Equation**

$H \Psi = E \Psi$

Cohesive energy, Lattice parameter

Bulk modulus, Electronic properties

Magnetic Properties etc …

**Monte Carlo**

**Δ**

**atomic group (# of valence e -)**

- 2nd period
- 3rd period
- 4th period
- 5th period
- 6th period
Molecular Dynamics Simulation

- Thin Film and Surface Phenomena in Atomic Scale

  - Asymmetric Intermixing of Interface
    - 0.1eV Al at 300K
    - 0.1eV Co at 300K

  - Surface Structure Evolution by Ion Bombardment
    - 10 keV Ar ion impacts on Au(001)
    - Atomic scale composition separation in CoCu alloy by Ar bombardment

  - Morphology Evolution of Nanoscale Materials
    - Al deposition behavior on Cu (111)
    - Stable phase in nanocluster is governed by the surface energy.
    - CNT buckling by sonication (in collaboration with Brown Univ.)

  - Origin of Stress in Amorphous Carbon Film