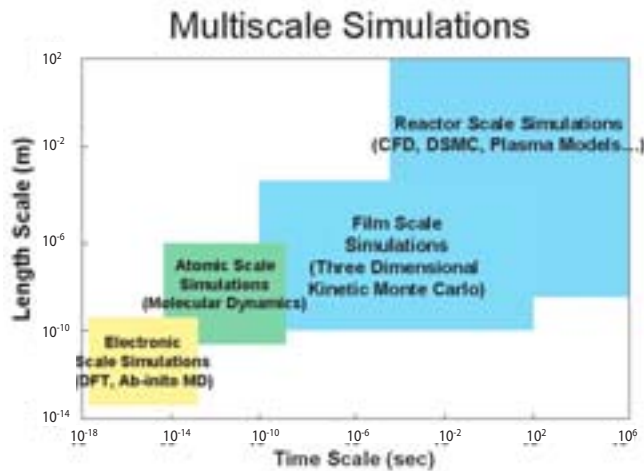


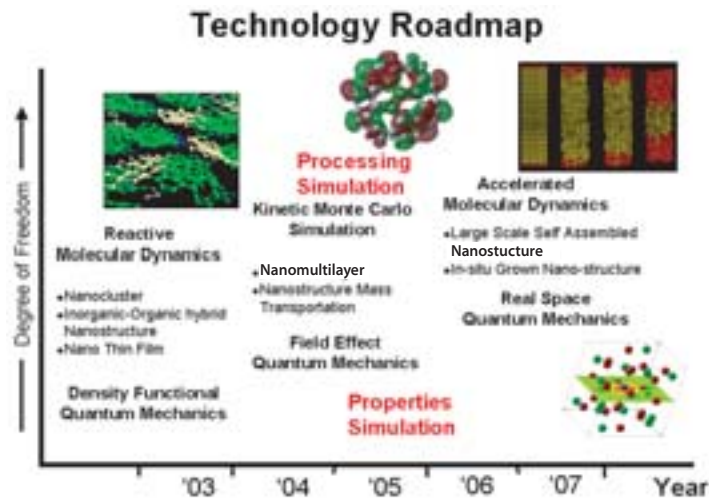
Nanostructure Simulation 奈米結構模擬

A multi-scaled simulation capability is critical to the realization of advantages of nanotechnology. ITRI is pursuing a hierarchical integration of continuum theory, molecular dynamics and ab initio quantum approach, so that explorations of compositions and structures can be conducted at various levels.

結合連續體理論、分子動力學及量子力學，建立奈米科技發展所需之多尺度模擬技術。



Technology Roadmap



Facilities

- Hardware**
- Beowulf Cluster (16 Dual CPU nodes + Myrinet, 16 nodes + GigaEthernet)
 - SGI O2 Workstation
 - DEC Workstation
 - PC Workstations (Linux *4, Win *4)
- Software**
- DL_POLY (Parallel Molecular Dynamics)
 - VASP (Parallel Ab initio Molecular Dynamics)
 - WIEN2k (Parallel Ab initio Molecular Dynamics)
 - ADF & BAND (Parallel Quantum Chemistry)
 - YFLOW (Parallel Fluid Dynamics)
 - Gaussian 98, MOPAC 2002, ANSYS...



Size Dependent Melting Temperature of Silicon Nanocrystal

