

Development of large-scale DFT method and its applications on nano-scale materials

Keywords: Density Functional Theory, O(N) method, nanoscale materials

Tsuyoshi Miyazaki

MANA Principal Investigator, Nano-Theory Field / First-Principles Simulation Group
 MIYAZAKI.Tsuyoshi@nims.go.jp | <http://www.nims.go.jp/cmsc/fps1>



Background

- First-principles method based on density functional theory (DFT) is a powerful tool, which can calculate the atomic and electronic structures without experimental information.
- But, usual DFT methods cannot treat the complex large systems, such as the interfaces in the actual materials or nano-structured materials.

Aim

- Development of a new calculation method called linear-scaling or O(N) method.
- Study of atomic and electronic structures of nano-scale materials and their complexes.
- Various theoretical analyses using large-scale first-principles molecular dynamics.

Advanced Research Topics

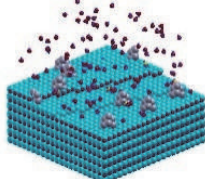
Large-scale DFT calculations using a linear-scaling method.

- DFT calculations on million-atom systems.
- Determination of the structure by structure optimization.
- Study of reactions or Structural Search by DFT-MD.

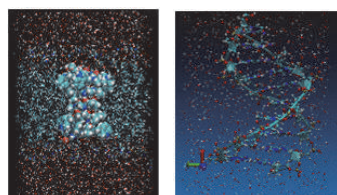
Nano islands in semiconductor surfaces



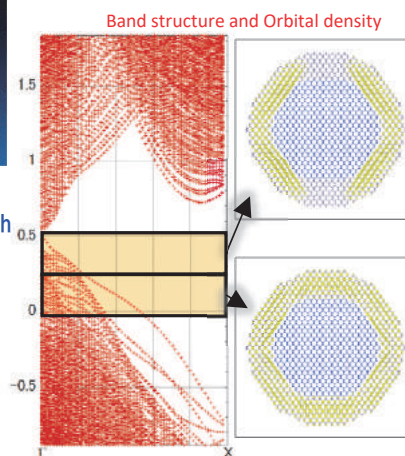
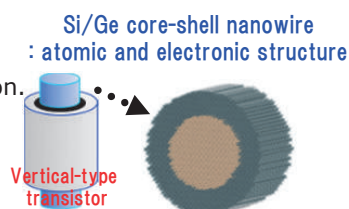
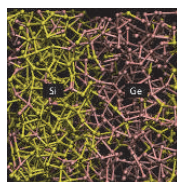
Catalysts of metallic nano-particles



Ion channel and DNA: dynamics



Si/Ge interface: structural search



Publications

- A. Nakata, Y. Futamura, T. Sakurai, D. R. Bowler and T. Miyazaki, J. Chem. Theory Comput. 13 (2017) 4146.
- T. Hirakawa, T. Suzuki, D. R. Bowler, T. Miyazaki, J. Phys. Condens. Matter 29 (2017) 405901.
- T. Suzuki, R. Tamura, T. Miyazaki, Int. J. Quantum Chem. 117 (2017) 33.

Summary

- Large-scale DFT simulations (up to million atom systems)
- Calculation of atomic and electronic structures of nano-scale materials or complex interfaces.
- Our large-scale DFT code will be open to public.

Research outcome

- Large-scale DFT study of complex nano-structured materials.
- The code can be used in the researches of many other materials and in various fields.