Development and applications of Large-scale DFT method

Keywords: Density functional theory, electronic structures, metallic nanoparticles

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Background

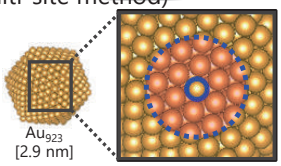
- Importance of simulation for materials design
- Size-restriction of accurate simulation because of computational cost
- A new approach for accurate simulation of large systems is needed

Aim

- Development of accurate and efficient technique for large-scale DFT simulations
- Efficient analysis method for electronic structure of large systems
- Applications of these methods on materials in realistic environment

Advanced Research Topics

Accurate large-scale DFT simulation
by using molecular-orbital like functions
(Multi-site method)



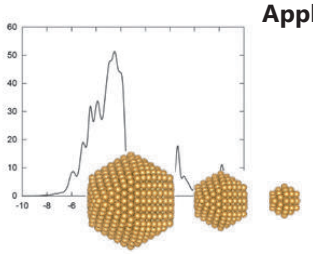
Au_{923}
[2.9 nm]

Development of large-scale DFT simulation method

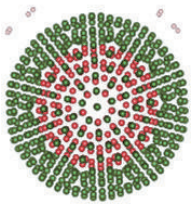
Electronic structure analysis of
Large systems
with Sakurai-Sugiura method

Charge distribution of Ge cluster on Si(001) surface (23,737 atoms) around Fermi level

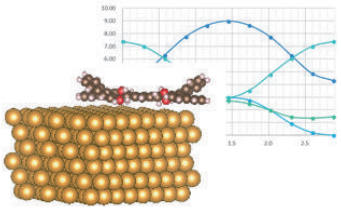
Applications on large-scale surface/interface



Site and size dependence of atomic and electronic structures of metallic nanoparticles



Atomic and electronic structure at surface and interface of core-shell nanoparticles



Analysis of the stability of molecules on metallic surface

Publications

- A. Nakata, Y. Futamura, T. Sakurai, D. R. Bowler and T. Miyazaki, J. Chem. Theory Comput. 13 (2017) 4146.
- A. Nakata, D. R. Bowler and T. Miyazaki, Phys. Chem. Chem. Phys. 17 (2015) 31427.
- T. Tsuneda, R. K. Singh, and A. Nakata, J. Comput. Chem. 38 (2017) 2020.

Summary

- Development of accurate and efficient calculation method
- Efficient analysis of electronic structure of large systems using Sakurai-Sugiura method
- Large-scale DFT simulation of metallic systems

Research outcome

- Multi-site method for accurate large-scale DFT simulation
- Efficient electronic structure analysis method for large systems
- Application on complicated surface/interface