Linear-scaling DFT simulations of complex nano-structured materials using the CONQUEST code

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First-principles simulations based on the density functional theory (DFT) are powerful tools to clarify the structural and physical properties of various materials at atomic scale. However, usual DFT methods cannot treat complex and large systems containing many thousands of atoms, since the calculation cost increases very rapidly, proportional to the cube of the number of atoms N in the system. To overcome this size limitation, we developed a linear-scaling, or O(N), DFT code CONQUEST. The code is based on the local orbital method and uses a density matrix minimization method to achieve the O(N) behavior. Using the code, we can treat large and complex systems containing more than 100,000+ atoms. We are planning to open the code with the MIT license soon.

In this talk, we will give an overview of the calculation methods used in the code, with its parallel efficiency on massively parallel computers. Then, we will present our recent study of nano-scale materials, Si/Ge or Ge/Si core-shell nanowires. We will show that CONQUEST can calculate the strain distributions in the actual size of the nanowires created experimentally, and unique electronic structure of Si/Ge or Ge/Si core-shell nanowires will be discussed. Some other applications using first-principles molecular dynamics will be also introduced.

This work was done in collaboration with Dr. J. Lin (NIMS) and Prof. D. R. Bowler (UCL). The code is developed jointly by the groups of University College London (D. R. Bowler), NIMS (TM, A. Nakata, Z. Raza, J. Lin, S. Yadav), and the University of Bordeaux (L. Truflandier). This work was supported by World Premier International Research Center Initiative (WPI Initiative) on Materials Nanoarchitectonics (MANA), New Energy and Industrial Technology Development Organization of Japan (NEDO) Grant (P16010), "Exploratory Challenge on Post-K computer" by MEXT, and JSPS Grant-in-Aid for Scientific Research (18H01143).

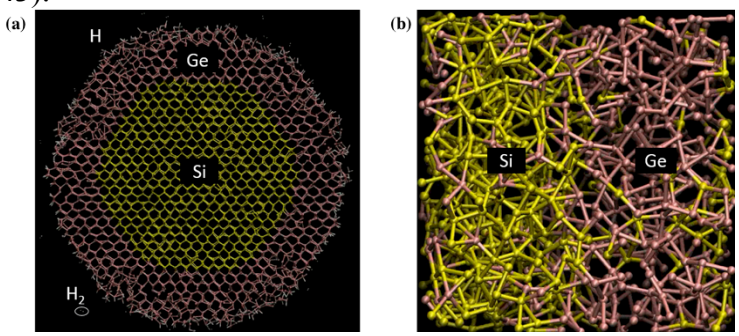

Figure 1: Snapshot structures of linear-scaling first-principles molecular dynamic simulations of Si/Ge core-shell nanowire (Left) and Si/Ge interfaces (Right)

References

1. D. R. Bowler and T. Miyazaki, *Rep. Prog. Phys*. 75, 036503 (2012).
2. http://www.linear-scaling.org