Center for Computational Sciences, University of Tsukuba
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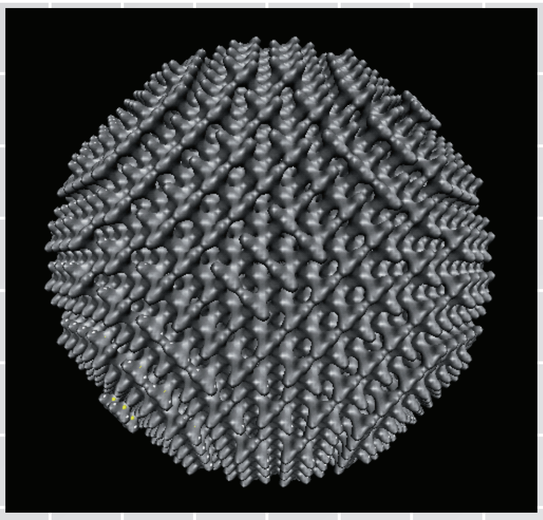
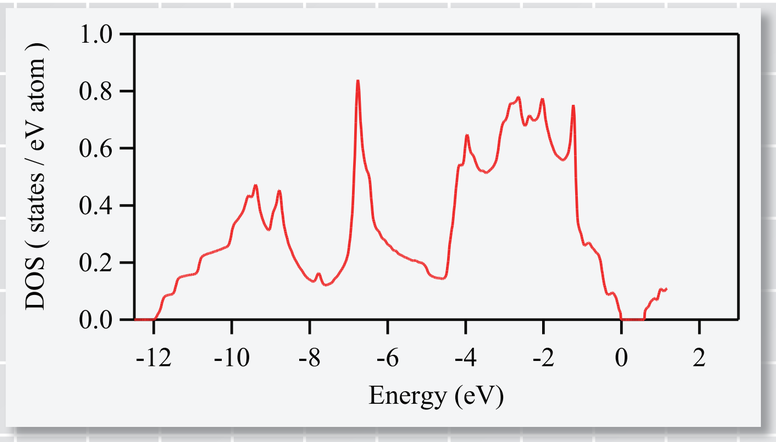
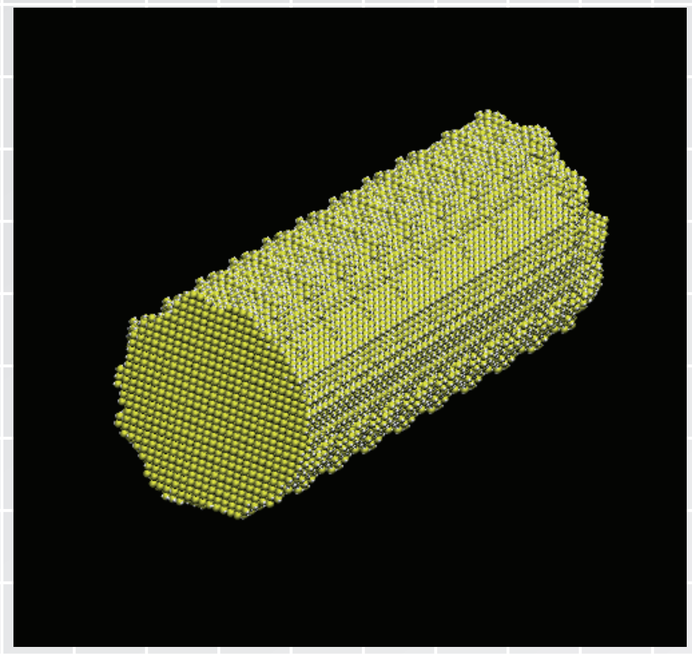
Materials Sciences on PACS-CS

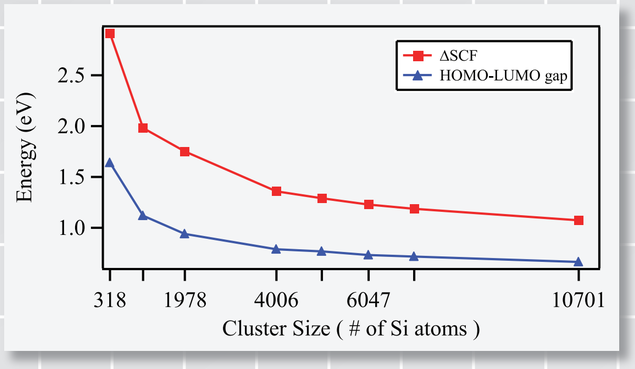
Large-scale electronic structure calculations for Si nanostructures

We have developed a quantum theoretical atomistic simulator based on the Real Space Density Functional Theory (RSDFT). In the RSDFT, all the calculations are done on lattices in real space. As a consequence, the scheme is free from the communication burden of the Fast Fourier Transform, utilize flexible boundary conditions, and is therefore best fitted to next-generation supercomputers with parallel architecture.



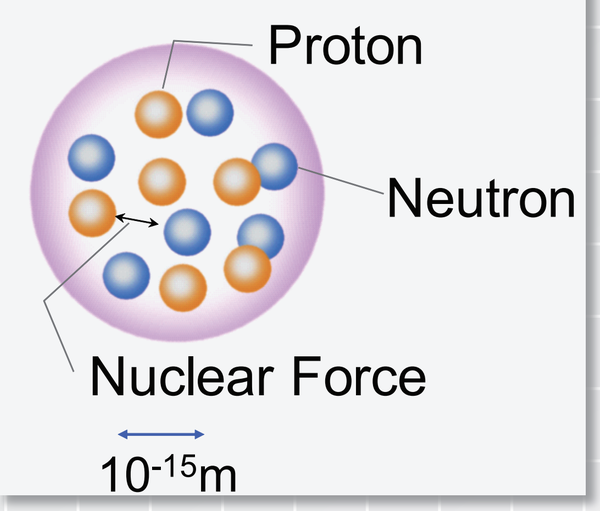






The targets of the RSDFT are nanostructures consisting over 10,000 atoms. We have achieved the calculations for a quantum Si nano dot consisting of 12,697 atoms and a rough Si nanowire consisting of 14,366 atoms within a few hundred hours by utilizing 1024 nodes of the PACS-CS. From these calculations, we can study the system size dependence of the band gaps, density of states, etc. for a wide range of the length scales, and we can also study the similarities and differences between the large-size nanostructures and their infinitely large size limit, namely the bulk materials.

Time-Dependent Density-Functional Theory



Atomic nucleus is an extremely high density matter located at the center of each atom. It is composed of protons and neutrons and is governed by the law of quantum mechanics. About 270 stable and 7,000 unstable nuclei exist in nature, and more than 3,000 nuclei have been synthesized artificially. To explore the properties of atomic nuclei in whole nuclear chart, a large scale computation based on the nuclear density functional theory has been successful.

The right figure shows a systematic calculation of the nuclear giant dipole resonances calculated at PACS-CS with the time-dependent density functional theory. The profile reflects the nuclear shape, and the strength is important to understand the origin of matter in the universe.