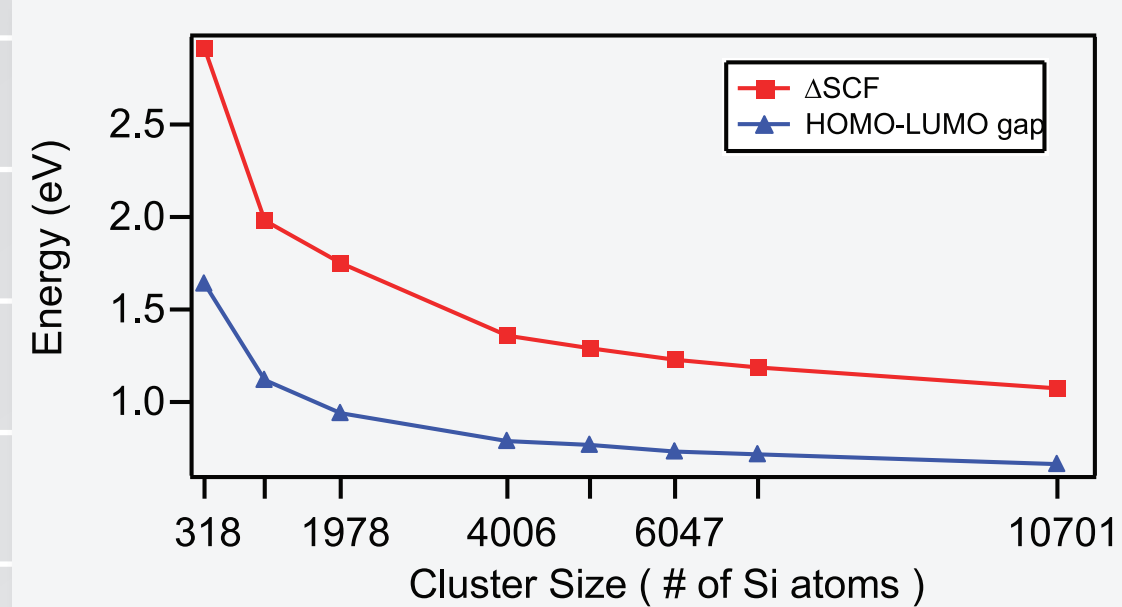
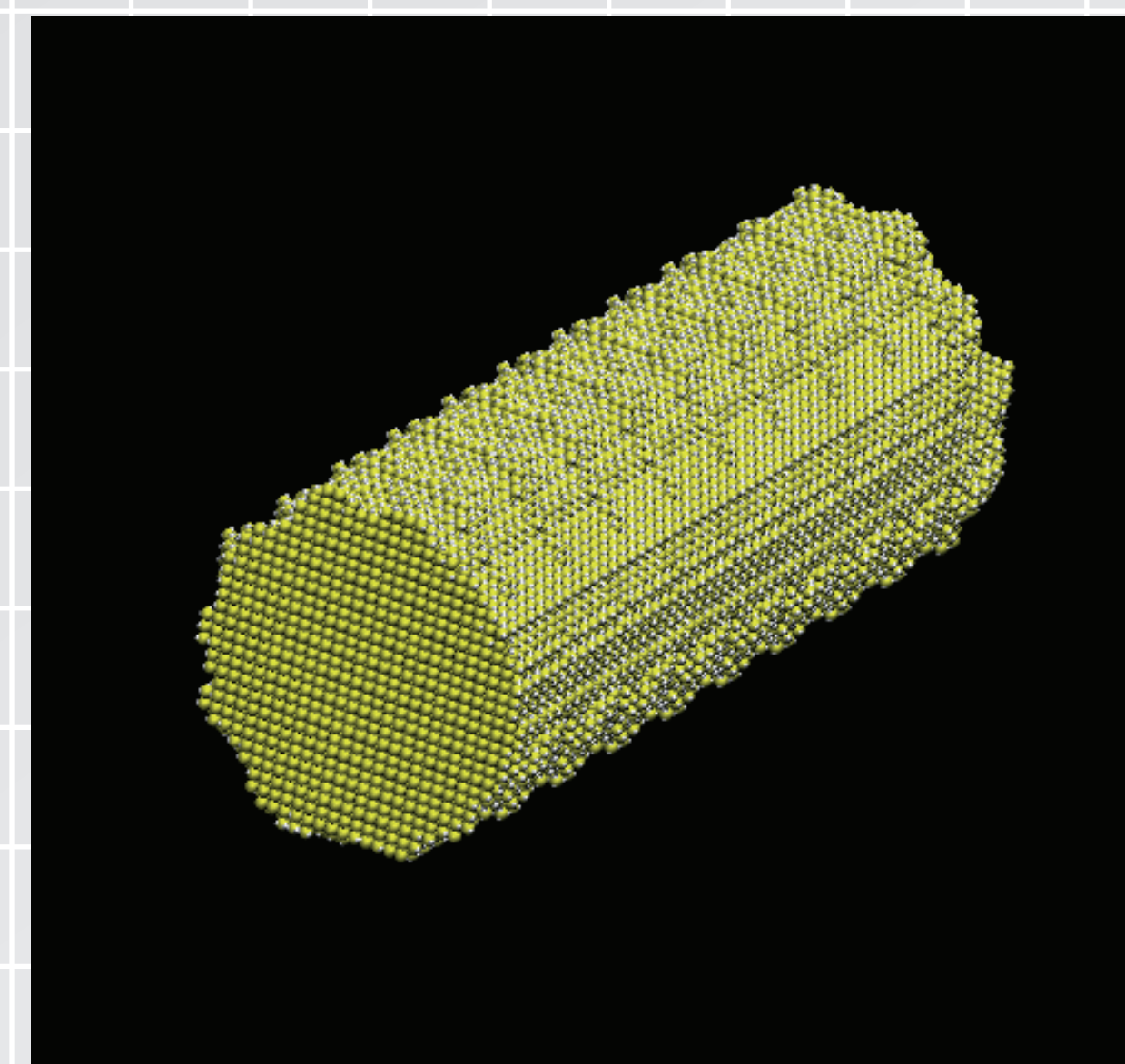
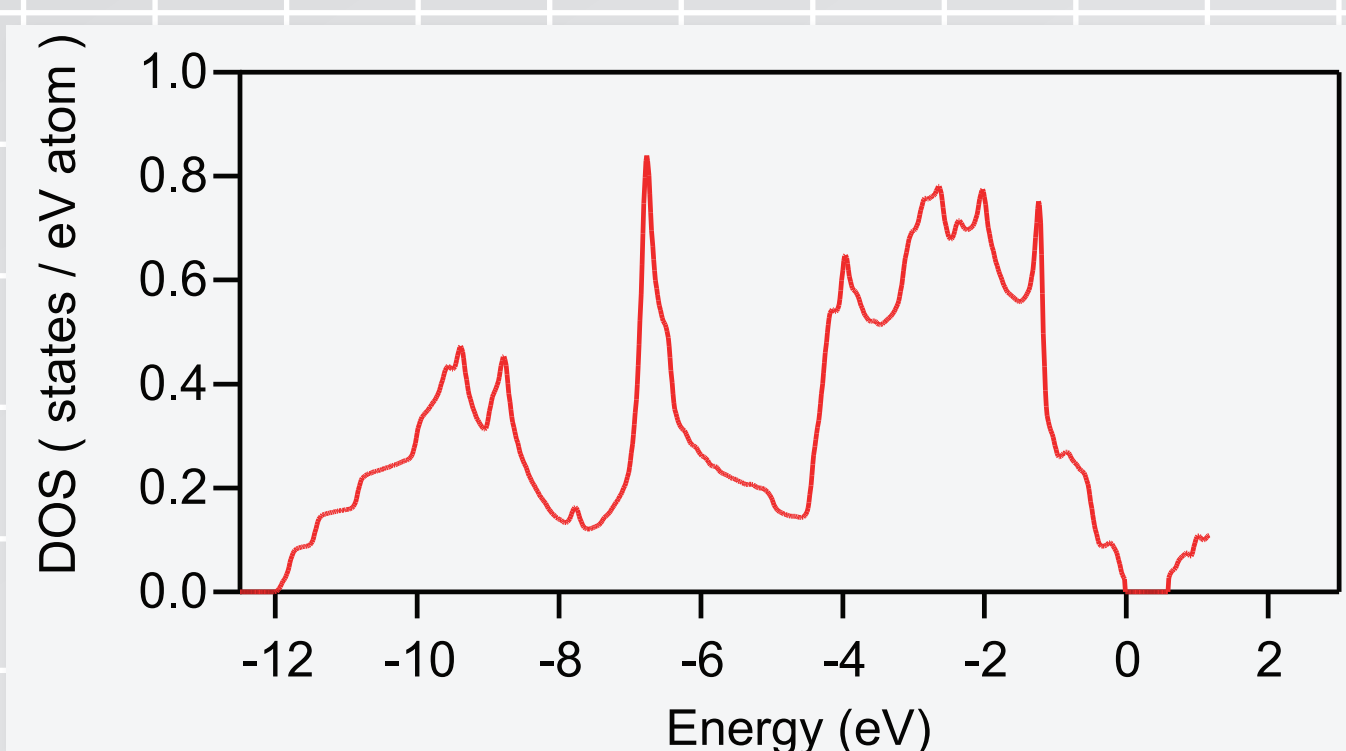
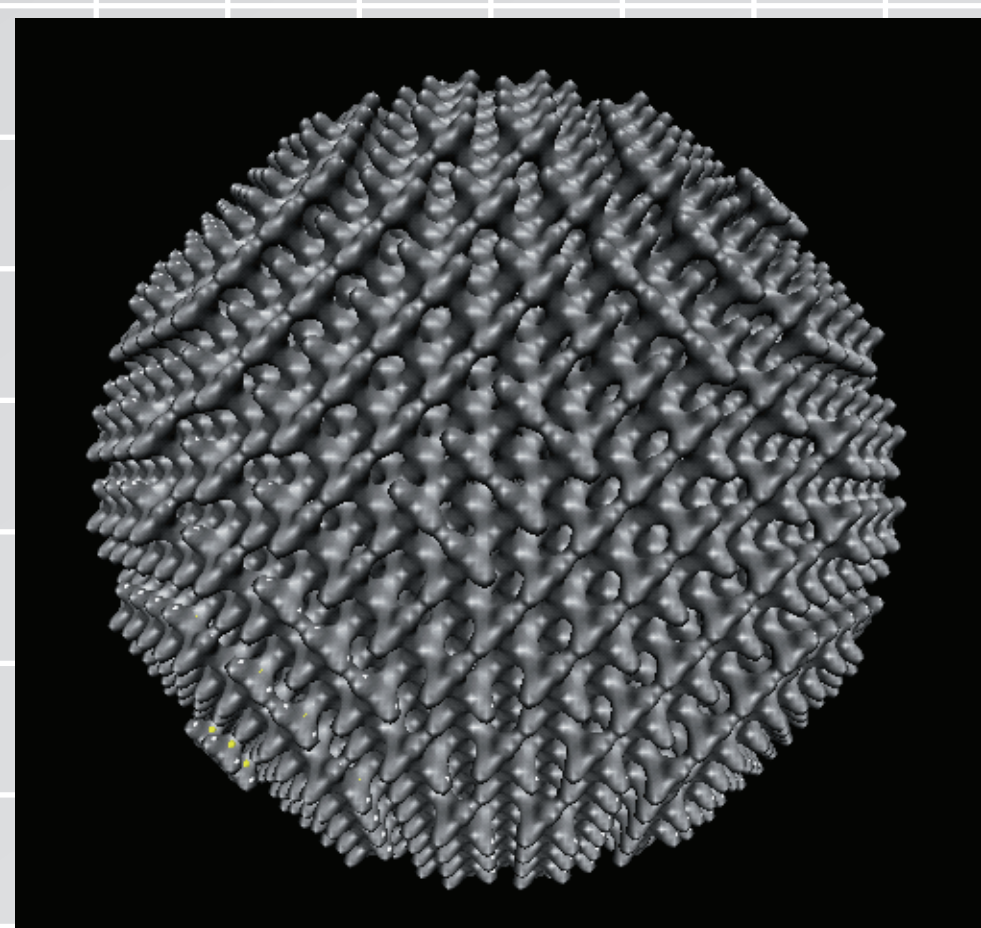


Materials Sciences on PACS-CS and T2K-Tsukuba

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, utilizes flexible boundary conditions, and is therefore best fitted to next-generation parallel architecture supercomputers.



The targets of the RSDFT are nanostructures consisting over 10,000 atoms. We have computed 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.

First-principles simulation for electron-phonon dynamics in solids

Time-dependent density functional theory (TDDFT) is an extension of the ordinary density functional theory for time-dependent electron dynamics. We have been developing a real-time and real-space method to solve the time-dependent Kohn-Sham equation. The method provides unified descriptions for diverse phenomena accompanying electron dynamics in linear and nonlinear regimes.

One of the subjects under intensive application of the TDDFT is the nonlinear electron dynamics induced by a strong and ultrashort laser pulse. Recently we have created a simulation to explore the mechanism of coherent phonon generation, a coherent atomic vibration induced by short laser pulses, and have succeeded for the first time to elucidate the mechanism in the first-principles calculation. The left-bottom figure shows the electric fields, and the right-bottom figure shows the force acting on atom. Across the direct band gap, a drastic change of phonon generation mechanism was observed. The right panels show electron densities in the ground state, a change of the electron density from ground state density during and after the laser pulse.

