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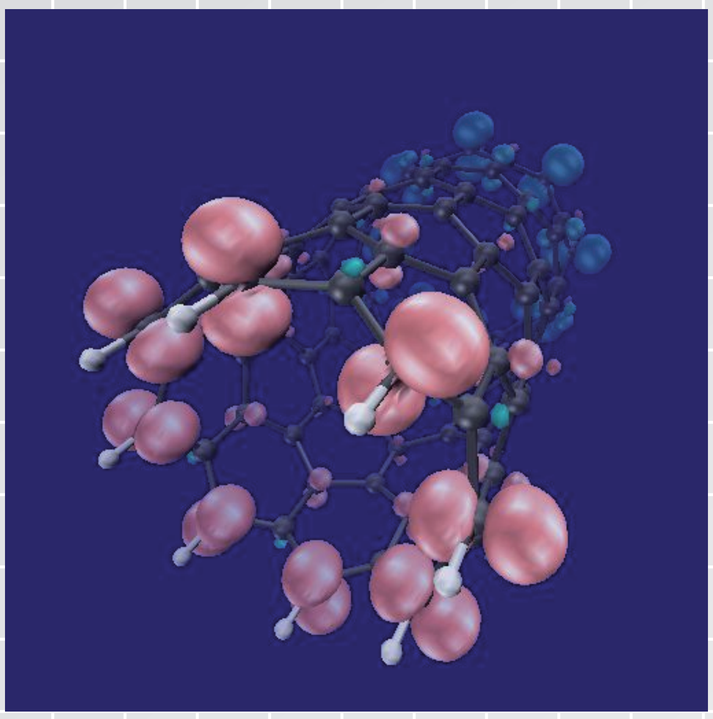
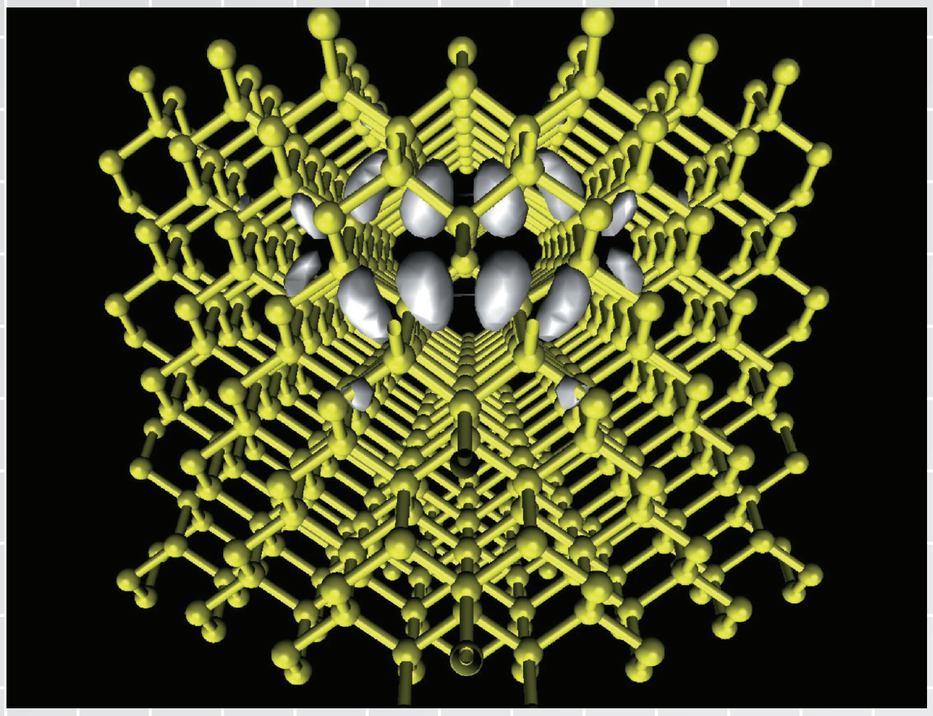
Computational Material and Life Sciences II

Real-Space Density-Functional Theory

We have developed a new scheme of quantum theoretical atomistic simulations based on the Density Functional Theory (DFT). In the scheme, all the calculations are done on lattices in real space. As a consequence, the scheme is free from the Fast Fourier Transform task, utilize flexible boundary conditions, and is therefore best fitted to computers with parallel architecture. The target is a nanostructure consisting of 10,000 atoms where new properties such as magnetism in carbon nanotubes (as predicted by our DFT calculations; Figure) may come up.





The new scheme, occasionally called Real-Space Density-Functional Theory (RSDFT) is first applied to clarify atomic structures of lattice vacancies in Si. There has been a long controversy as to accurate atomic arrangements around a divacancy. The figure shows the determined structure of the divacancy and corresponding electron cloud nearby. Accurate structural determination is necessary to identify electronic properties of nano Si.

Electron dynamic induced by intense laser field

Intense short-pulse laser field induces a variety of nonlinear phenomena reflecting electron dynamics in femtosecond time scale. We study them with the time-dependent density-functional theory solving the time-dependent Kohn-Sham equation in real-space and real-time. The figure shows the electron dynamics in Ar atom where the electron emitted from an atom and accelerated by the laser field collides with the atom. This process is called the electron rescattering, and is used as a source of short-pulse X-ray.