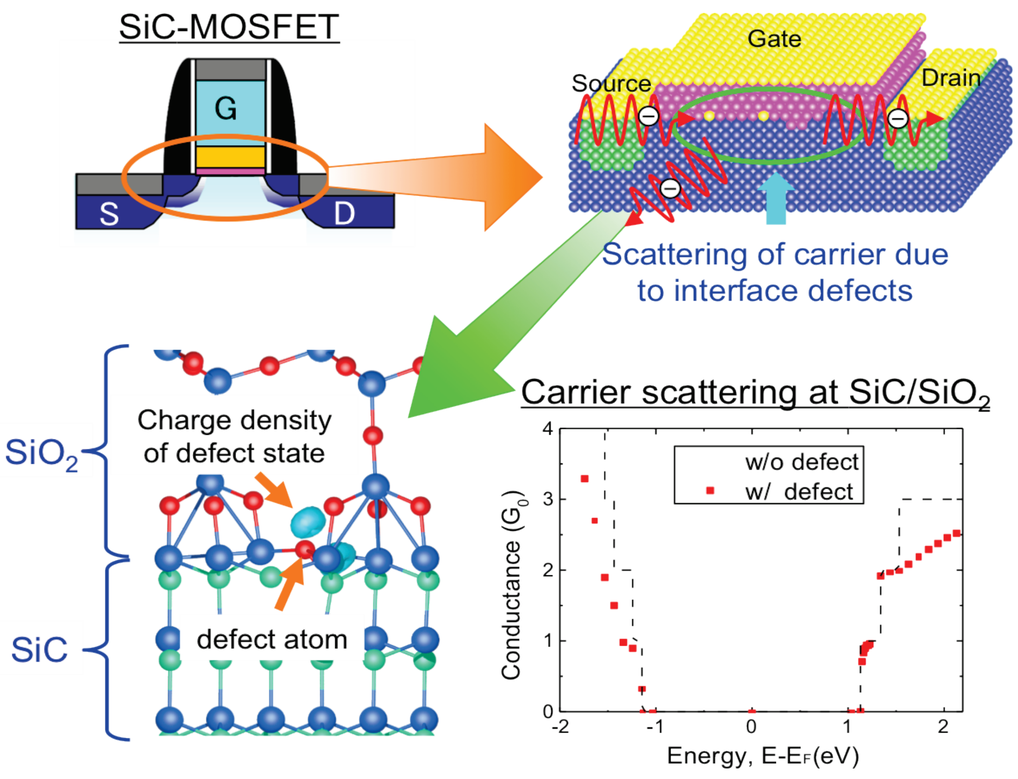
Quantum Condensed Matter Physics

Computational Design of Future Electronics Devices using First-Principles Calculations

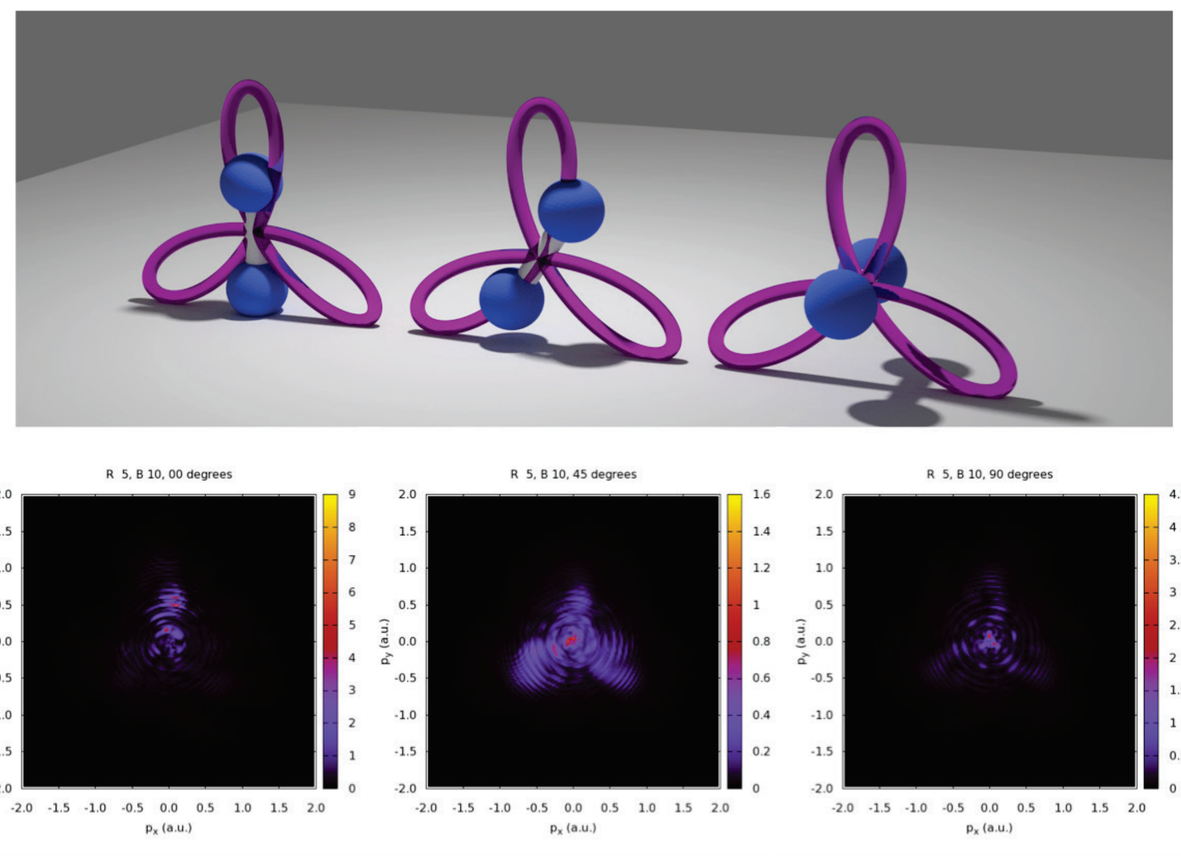
A typical trend in first-principles electronic-structure calculations is that we deal with increasingly complex systems characterized by many atoms of different chemical nature in open structures and of low symmetry. This path is supported by the increasing availability of increasingly powerful computers spearheaded by high-performance computers. The developments of the latter show that we have to cope with massively parallel computer architectures dealing with thousands of cores. This path accelerates in the next 10 years with the attempt moving from peta-scale to exa-scale computing. Thus developing electronic structure methods whose applicability scales with the available processes becomes a prerequisite.



We develop first-principles calculation code “RSPACE.” RSPACE is based on the real-space finite-difference method, which is an approach that has the potential to scale with massively parallel architectures and has this potential without compromise on the precision and it should be superior to conventional plane wave methods. As applications using RSPACE, interface atomic structures and fabrication procedures are developed using first-principles calculations to realize high-performance and low-energy-loss electronic devices, e,g., SiC power devices. By investigating the origin of leakage current and carrier scattering at interfaces, we propose prescriptions to improve device performance and demonstrate the applicability of the interface structures. Furthermore, we establish a basic technology of computational science to design interface structures and fabrication procedures of future electronic devices.

Time-Dependent Method for Isolate Many-Atom Systems in Intense Laser Fields

Isolate many-electron systems, like atoms, molecules and clusters, in an intense laser field are the current hot topics because the processes can be used to generate atto-second (10^{-18} s) pulses, image the molecular structure, and push the femto-chemistry into atto-chemistry. Unfortunately, such a process cannot be observed directly from experiments. The detailed dynamic information can only be dug out by comparing the first-principles simulation with measurements. The characteristics of many-atom systems in an intense laser field are that many continue states are involved and the ejected electron can go far away from its parent core and return to the core again at a later time. Thus the conventional quantum-chemistry codes, like BigDFT or GAMESS, do not work in the intense laser material interactions although they are popularly used for the structure and spectrum calculations.



To cope with the characteristics of the problem, we develop a time-dependent Schrödinger equation solver for many-electron systems based on the density functional theory. Real space in a rectangular box is discretized with an equal space grid and the time-propagation is performed with a second-order-split-operator method by using the fast-fourier-transformation. The advantages of the new method are that the unitary of electron wavefunctions is automatically satisfied and the numerical precision can be controled by tuning the time-step. More important, the method can be used for a large system with the number of grid point more than handred millions. The above figure shows a test run of the electron momentum distribution of N_2 molecules in two-color count-rotating circularly polarized laser fields with different aligment angles between the polarization plane and the molecular axis. The grid points used in the simulation are 1000x1000x100 in a rectangular box. The new method is expected to work in a more complex many-electron system in intense laser fields.