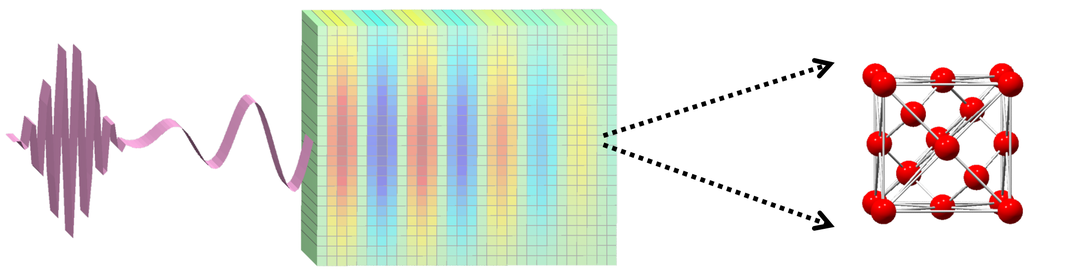
Quantum Condensed Matter Physics

SALMON: Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience

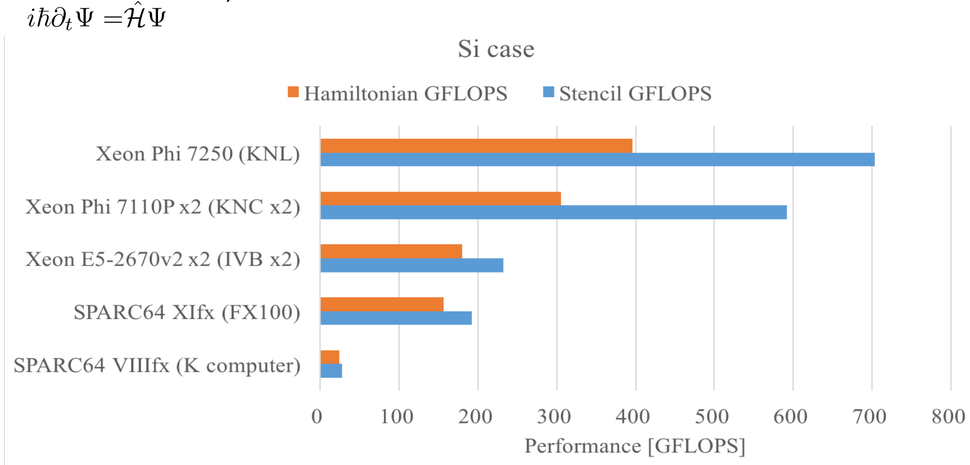
Interactions between light and matter are the basis of a wide range of technologies. To gain a basic understanding of the interaction, it is essential to realize electron dynamics in matter induced by the light electromagnetic fields in a microscopic scale, 10^{-9} (nano-)meter in space and 10^{-15} (femto-) second in time. We have been developing a computer code SALMON, Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience, under a collaboration with researchers in Institute for Molecular Science. It is based on time-dependent density functional theory in microscopic scale. SALMON is available at http://salmon-tddft.jp.



Macroscopic system (Electromagnetics)
$\left(\nabla^2 - c^{-2}\partial_t^2\right)\mathbf{A} = -4\pi\mathbf{J}/c$

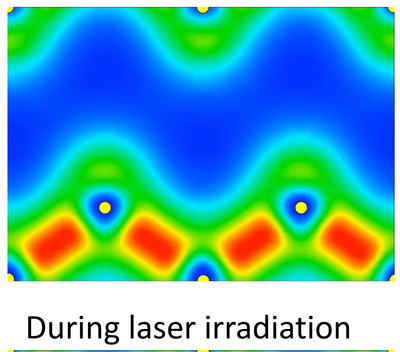
Microscopic system (Quantum mechanics)
$i\hbar\partial_t\Psi = \hat{\mathcal{H}}\Psi$

SALMON may describe coupled dynamics of electrons and electromagnetic fields in a multiscale modeling. In microscopic scale, time-dependent Kohn-Sham equation is solved in real space grid representation. Maxwell equations for the light electromagnetic fields are solved employing finite-difference time-domain method.

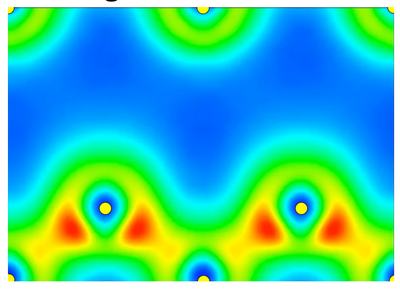


SALMON is optimized for latest processors of different architectures. Performances of SALMON (Hamiltonian and stencil operations) are compared.

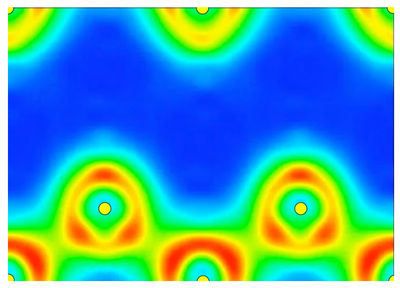
Ground state



During laser irradiation



After laser irradiation



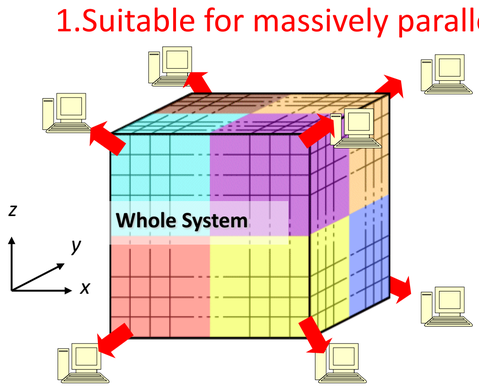
Electron motion in crystalline silicon induced by intense and ultrashort laser pulse.

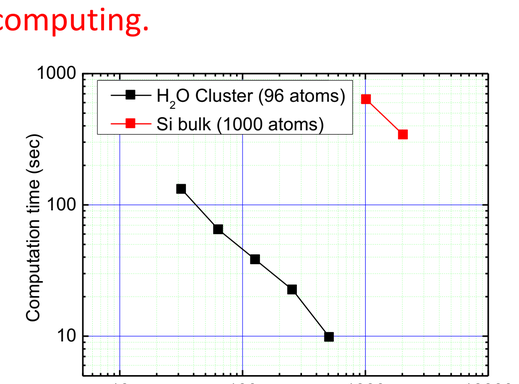
Computational Design of Future Electronics Devices using First-Principles Calculations

With cutting-edge materials and minute electronic devices being produced by the latest nanoscale fabrication technology, it is essential for scientists and engineers to rely on first-principles calculations to fully understand phenomena from the behavior of electrons. We develop first-principles calculation code "RSPACE."

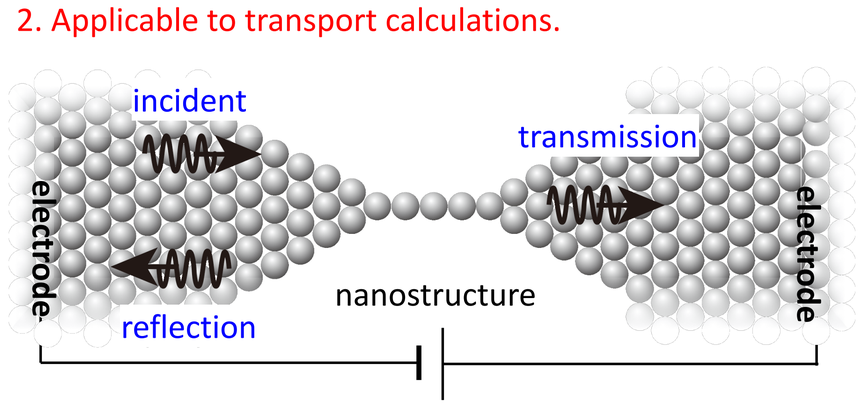
RSPACE uses real-space finite-difference method for first-principles calculation. The advantages of RSPACE, which are superior to conventional plane wave methods, are

1.Suitable for massively parallel computing.

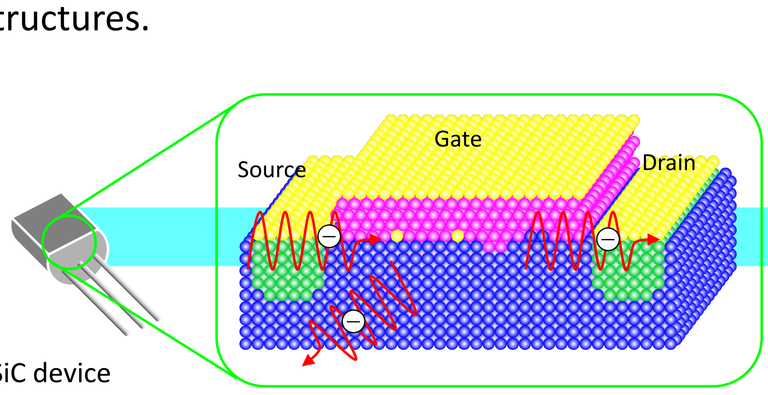




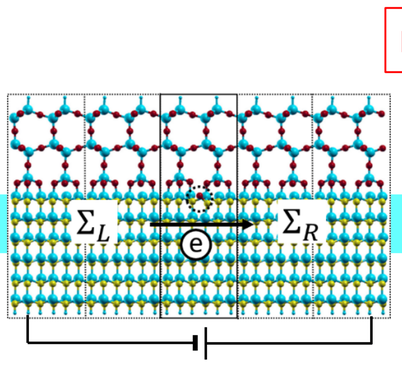
2. Applicable to transport calculations.

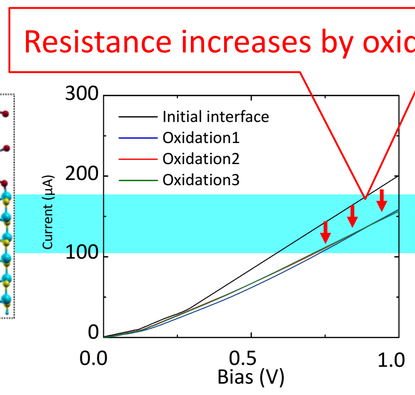


As applications using RSPACE, interface atomic structures are examined and fabrication procedures are developed to realize high-performance and low-energy-loss electronic devices, e,g., SiC power devices. By investigating the origin of leakage current and carrier scattering at interfaces, we propose prescriptions to improve device performance and demonstrate the applicability of the interface structures.

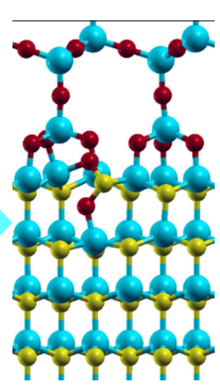


Scattering of carrier due to interface defects





Carrier scattering property obtained by RSPACE.



Computational design of interface structure

Furthermore, we establish a basic technology of computational science to design interface structures and fabrication procedures of future electronic devices.

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