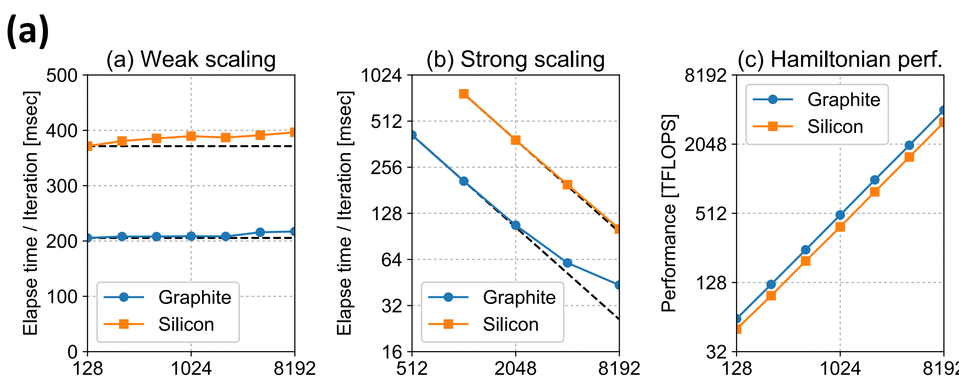
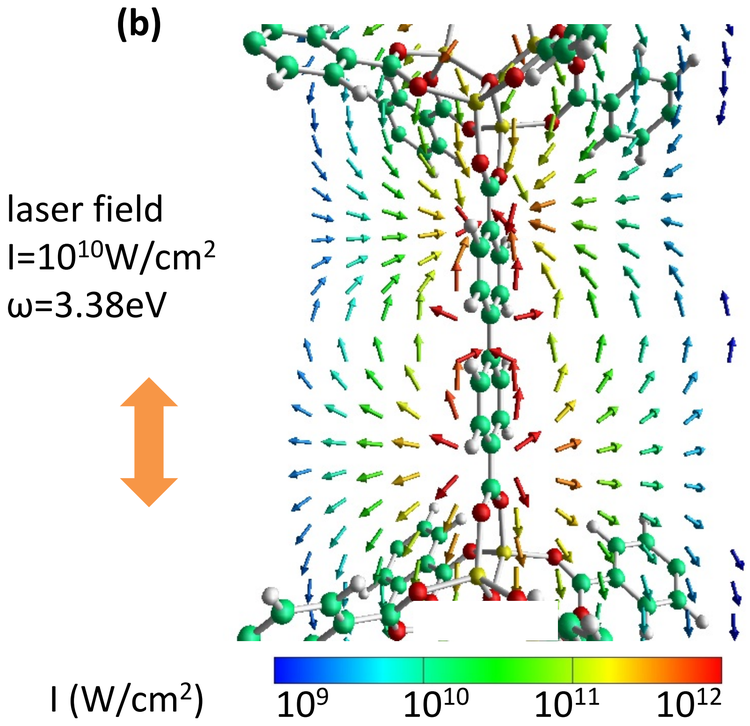
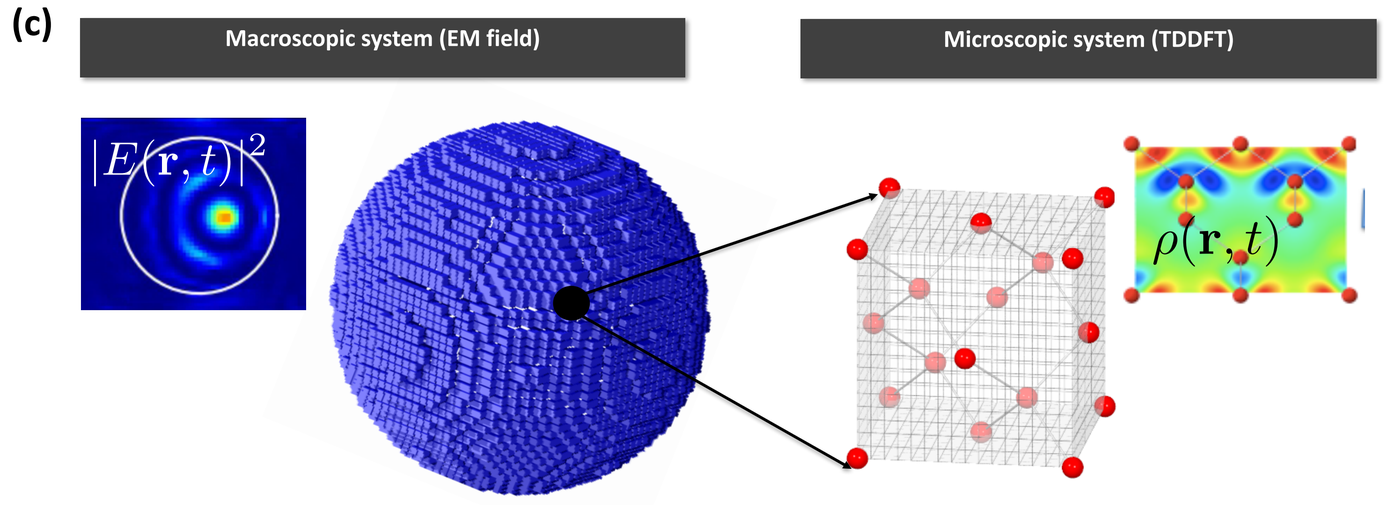
Quantum Condensed Matter Physics

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

Understanding interaction between light and matter is the basis of a wide range of technologies. For this purpose, it is essential to describe electron dynamics in matters induced by light electromagnetic fields in a microscopic scale, 10^{-9} (nano-)meter in space and 10^{-15} (femto-) second in time. We have been developing an open-source computer code SALMON, Scalable Ab-initio Light-Matter simulator for Optics and Nanoscience that describes electron dynamics in molecules, nano-materials, and solids based on first-principles time-dependent density functional theory [http://salmon-tddft.jp].







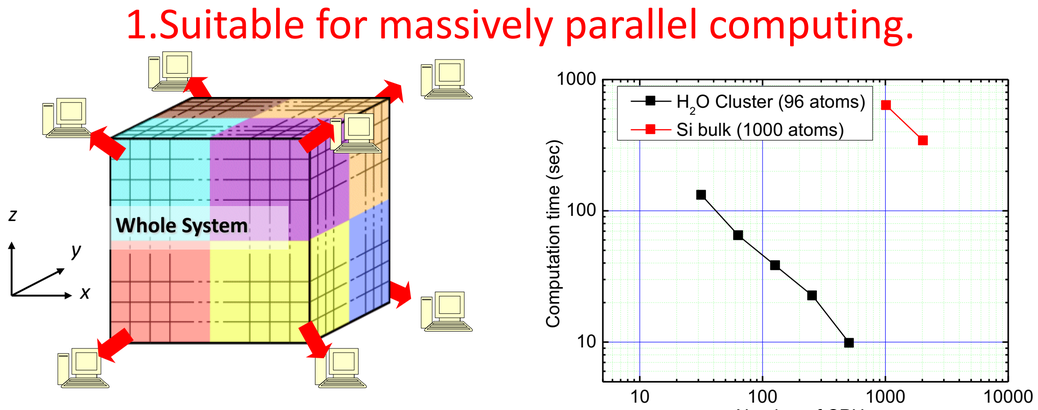
(a) Performance of SALMON using full nodes of Oakforest-PACS.
(b) Optical near-field generated in metal-organic framework, IRMOF10.
(c) Intense pulsed light irradiates on silicon nano-sphere of 250nm radius by coupled Maxwell-TDDFT calculation.

Computational Design of Future Electronics Devices using First-Principles Calculations

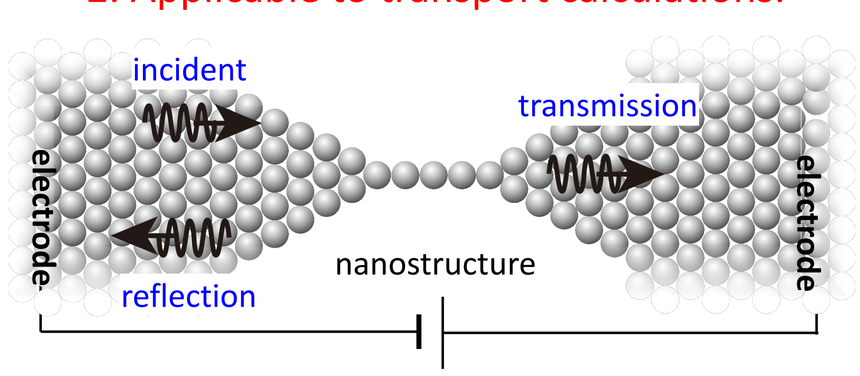
With cutting-edge materials and minute electronic devices being produced by the latest nanoscale fabrication technology, it is essential for scientists and engineers to rely on first-principles calculations to fully understand phenomena from the behavior of electrons. We develop first-principles calculation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

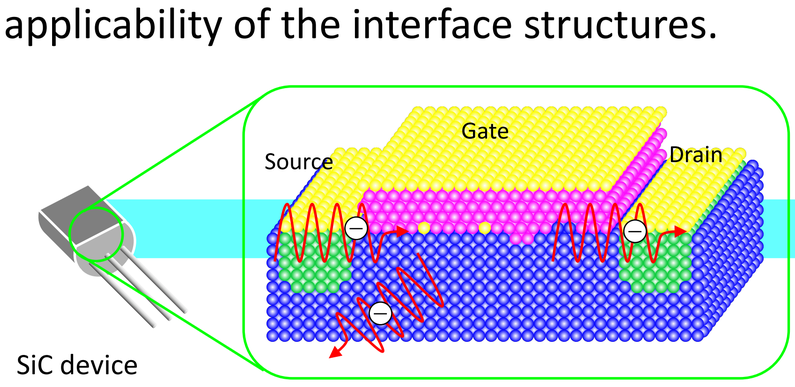
1.Suitable for massively parallel computing.



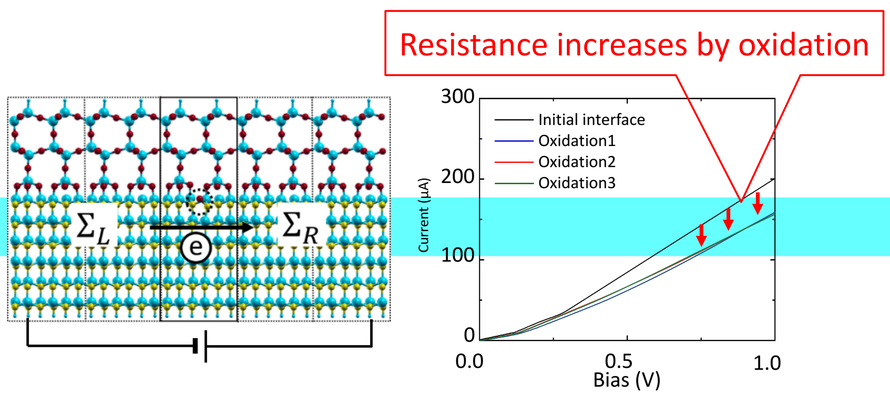
2. Applicable to transport calculations.



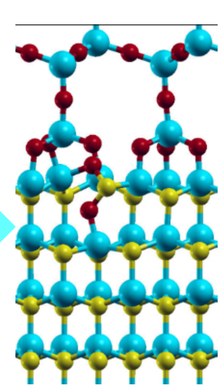
As applications using RSPACE, interface atomic structures are examined and fabrication procedures are developed to realize high-performance and low-energy-loss electronic devices, e,g., SiC power devices. By investigating the origin of leakage current and carrier scattering at interfaces, we propose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