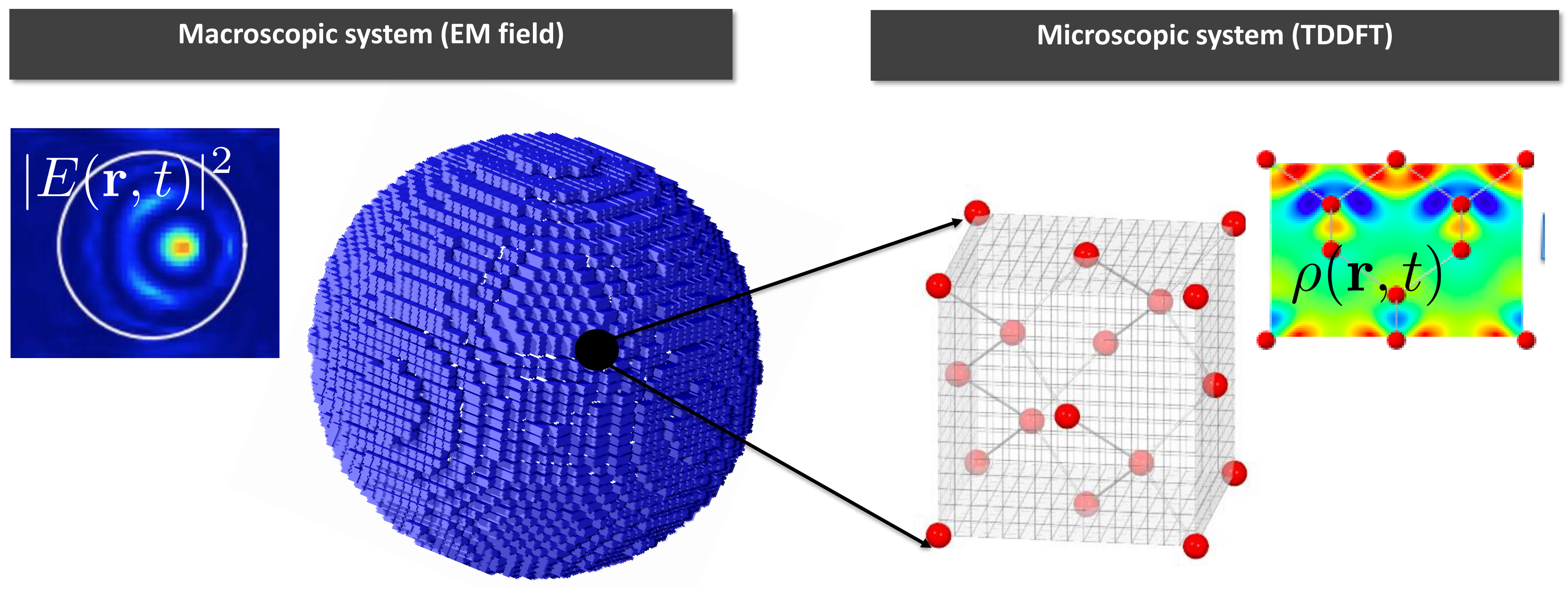
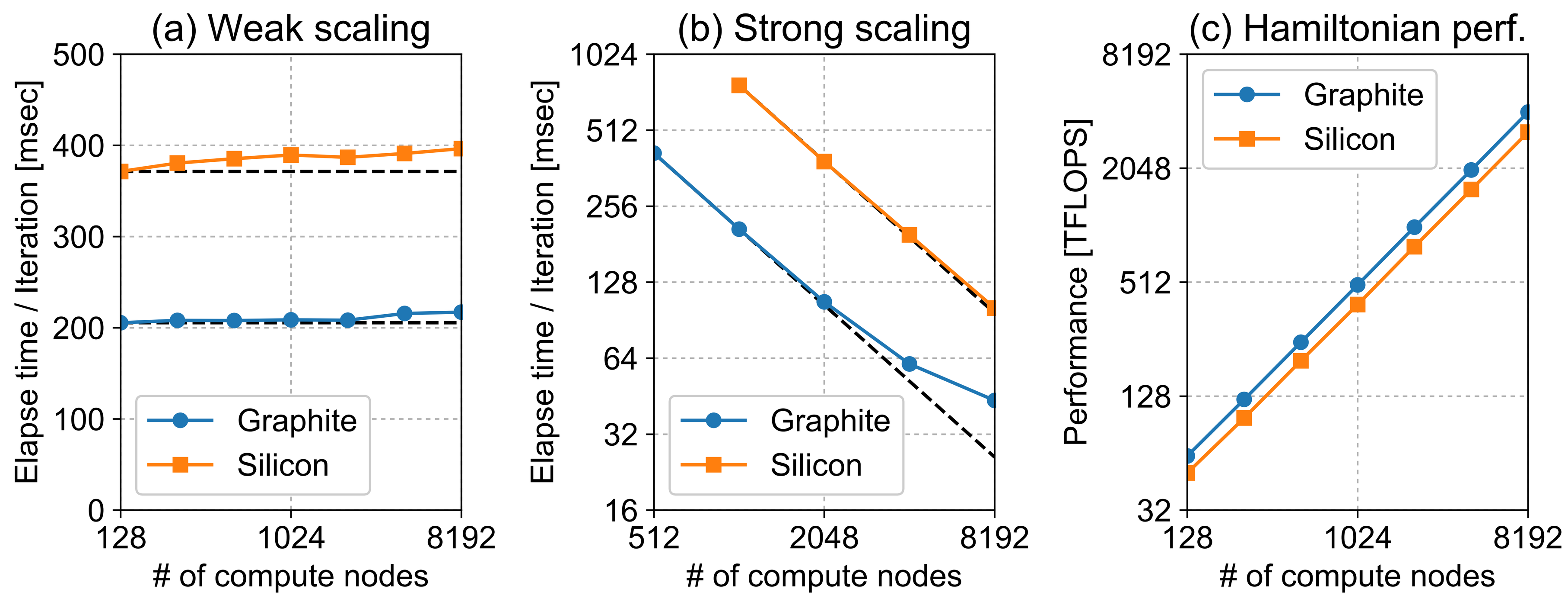
Quantum Condensed Matter Physics

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]. As a novel function of SALMON, light propagation in nano-materials as well as in bulk medium can be described taking full account of nonlinearity and nonlocality of light-matter interactions in the ab-initio level. We expect SALMON will be widely used in cutting-edge researches in optics and nanoscience.



(a) Maxwell-TDDFT multiscale calculation: Irradiation of an intense and ultrashort light pulse on silicon nanosphere of 250nm radius.

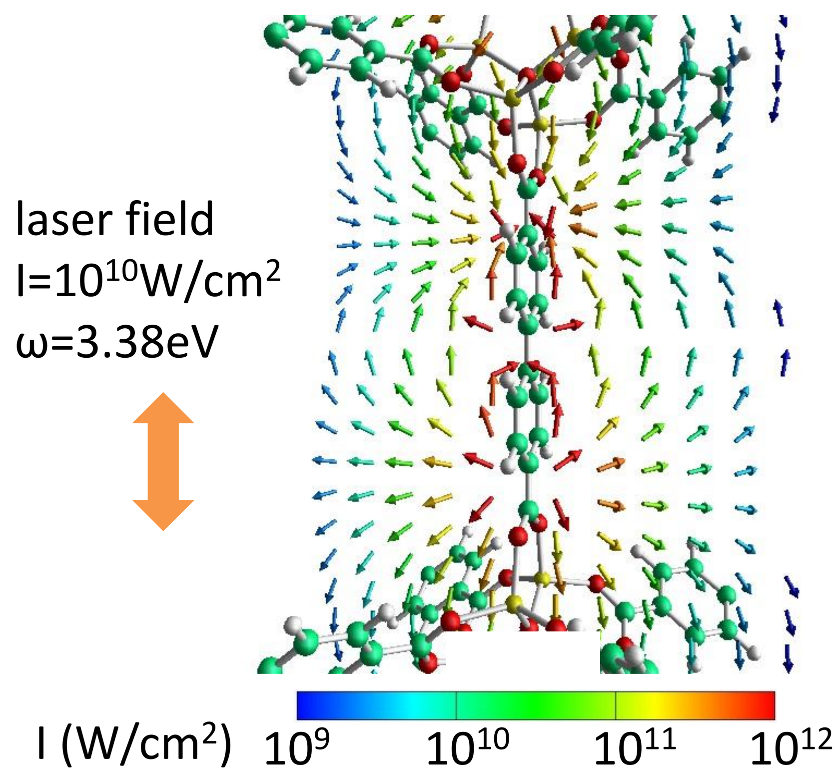


(b) Performance of SALMON using full nodes of Oakforest-PACS.

Optical Properties of Nano-materials in Real Time and Real Space

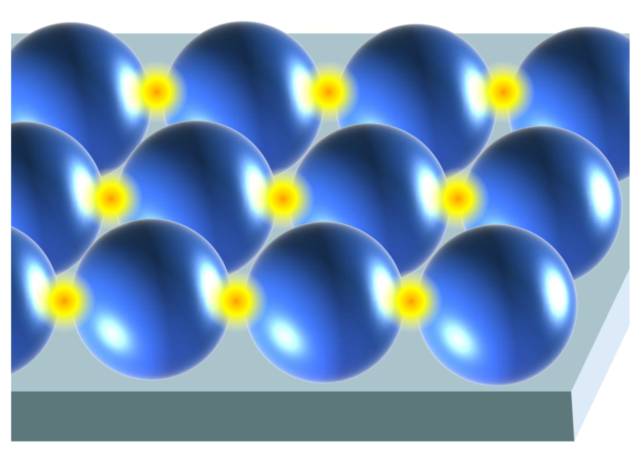
(a) Optical near-field generated in metal-organic framework, IRMOF-10

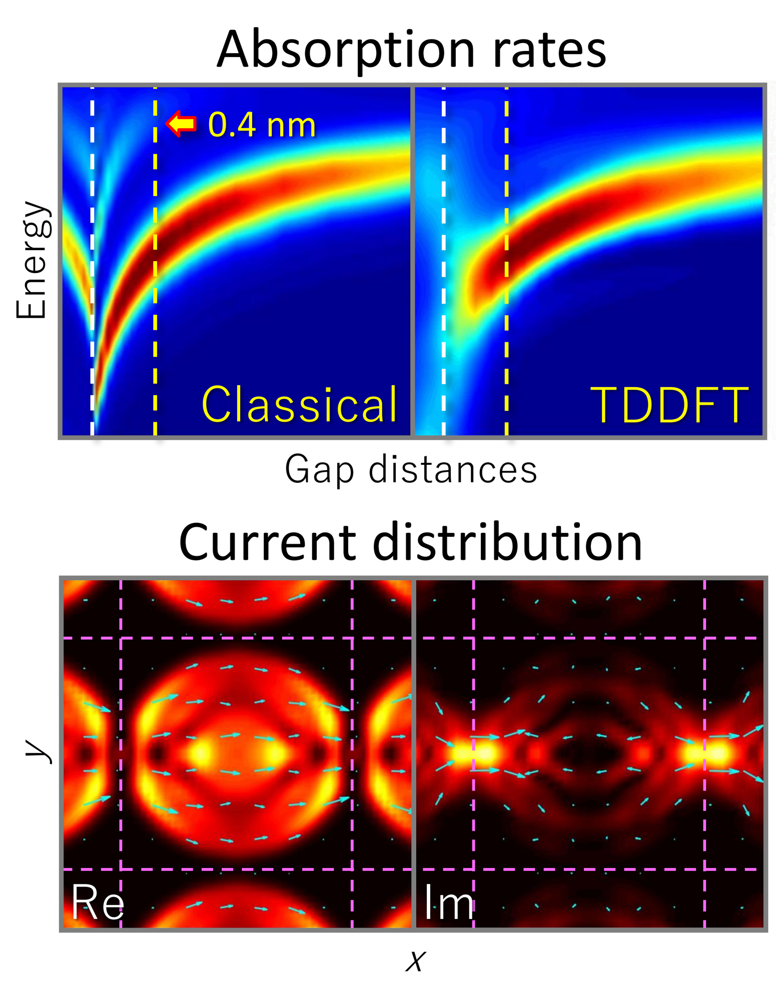
When a light pulse irradiates on nano-sized objects, a strong and spatially-localized electromagnetic field, which is called the near field, appears around the object. The near field enables imaging beyond the limit of optical resolution and enhances nonlinear optical processes. We perform first-principles calculations of the photoexcitation dynamics of an acetylene molecule in a metal organic framework, IRMOF-10. Resonant laser excitation of the IRMOF-10 generates an optical near field around the two benzene rings that comprise the main framework of the IRMOF-10. The second harmonic excitation caused by spatial nonuniformity of the optical near field is observed.



(b) Optical property of metallic metasurface with sub-nm gaps

By virtue of rapid progresses in fabrications of nano-materials, it is possible to manufacture periodic materials composed of uniformly structured nano-objects. Here we investigate the optical properties of quantum plasmonic metasurfaces composed of two-dimensional arrayed metallic nano-spheres with sub-nm gaps according to the time-dependent density functional theory, a fully quantum mechanical approach. When the quantum and classical descriptions are compared, the absorption rates of the metasurface exhibit substantial differences at shorter gap distances. The differences are caused by electron transport through the gaps of the nano-objects.





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