

CAMT Seminar

“Multiscale modelling of nanoscale materials and
electronic transport”

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Date: December 9, 2015 (Wed) 14:00-15:00

Location: Main Conference Room (1st floor), Bldg. A12
Center for Atomic and Molecular Technologies (CAMT)
(A12 棟 1 階会議室)

To support accelerating materials development cycles we have developed simulation approaches for de-novo characterization and optimization of materials and device properties with nanoscale constituents. In recent years we have therefore developed simulation methods that describe the conformation and electronic properties of materials built on the basis of well-defined nanoscale constituents. Here we discuss development of the atomic transistor, the electronic and structural properties of nanocarbon materials, and organic light emitting diodes. In the EU project MMM@HPC we have developed unified multi-disciplinary approach that integrates materials science simulation and high performance computing is required to transform isolated solutions for specific problems into comprehensive, industry-ready platforms, which are capable of predicting the properties of complex materials on the basis of their constitutive elements.

(Host: Satoshi Hamaguchi Ext:7913)