OIST

Nano Seminar

Date/Time : (Thu) 13th March / 15:00~16:00
Venue: Lab 1, Seminar Room C015, Main Campus
Speaker: Prof. Hiromitsu Takaba

Multi-Scale Modeling on Catalysis and Functional Materials

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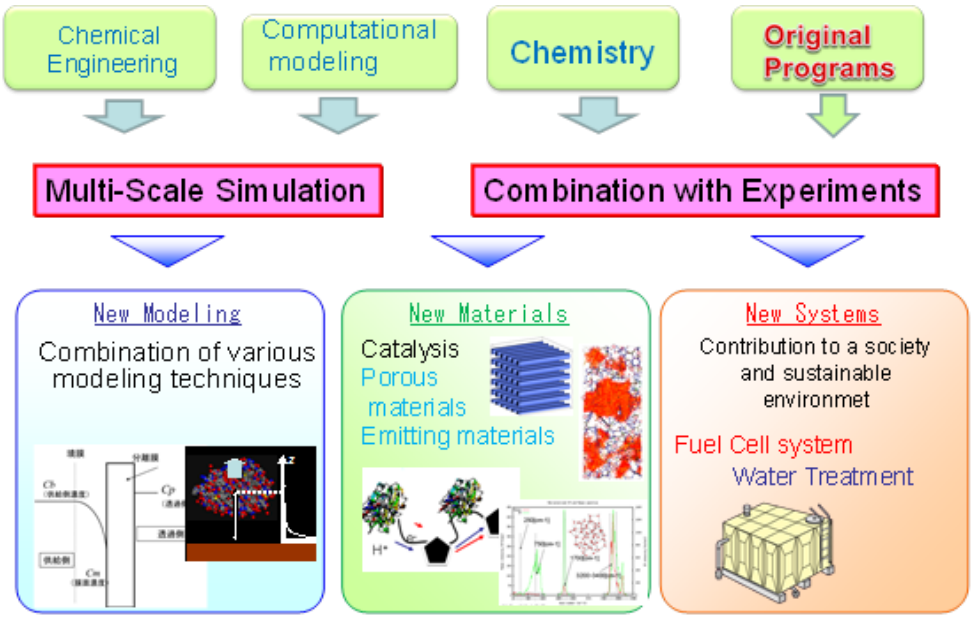
Abstract:

Recent applications of multi-scale computational chemistry to design of functional materials will be presented. Our multi-scale computational chemistry approach is on the basis of microscopic molecular simulation such as quantum chemistry calculation and molecular dynamics. The combination of them with alternative macroscopic modeling techniques, eg., computational fluid dynamics or chemoinformatics, enables to design of functional materials. In this presentation, the result of catalysis, gas reaction on precious metals for purification waste gas in automobile, modeling of degradation of precious metals in polymer electrolyte fuel cell, and design of novel oxide phosphor materials for light-emitting diode device.



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