The 681st

MANA & GREEN

The 77th

The 11th Joint Seminar

Nano Revolution for the Future

Toward a new simulation study of substance transportation in the inhomogeneous large systems – revisit at dynamic Monte Carlo method

Chair: Dr. Yoshitaka TATEYAMA (MANA PI / Deputy Director, GREEN)

Prof. Susumu Okazaki

(Graduate School of Frontier Sciences, The University of Tokyo, Japan)

Transportation of molecules in the inhomogeneous systems has been becoming very important in science and engineering. For example, in the fuel cells, four-phases electrode interface has a very complex structure formed by platinum, carbon, polymer electrolyte, and water. Hydronium ions, hydrogen molecules, and oxygen molecules migrate in the interface to reach the electrode. Scale of the inhomogeneity is great. It is in the order of sub microns. Further, bulk structure of the polymer electrolyte itself shows a very complicated and inhomogeneous one, where microscopic phase separation is found between polymer and water phases. The ions and molecules move through the water phase and polymer phase either. In this case, the scale of the inhomogeneity is in the order of nanometers. These systems are too large to investigate directly by molecular dynamic calculations when we are interested in the global diffusivity of the ions and molecules in them. Here, we discuss about our new strategy for the investigation of these systems, where we coarse grain them into a simple model and, after then, we trace the global diffusivity of the ions and molecules by dynamic Monte Carlo.

Venue: Auditorium, 1F, WPI-MANA Bldg., Namiki-site / Zoom (Hybrid)

Date: July 20th, Tuesday Time: 13:30-14:30

Registration form for Zoom on-line participation : https://forms.gle/xRcVe4tskBhRz7YA7

(Registration Closing Date: 12:00 PM on 19th July, 2021)

Contact: International Center for Materials Nanoarchitectonics (MANA)