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# Large scale molecular simulations for transport phenomena in polymer electrolyte fuel cell

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Polymer electrolyte fuel cell (PEFC) is expected to be a next power-supply system. In PEFC, water is generated from hydrogen and oxygen and electrical power is generated. To achieve higher performance of PEFC, the reaction materials, that is hydrogen, oxygen and water molecules, should transfer in Membrane Electrode Assembly (MEA) as fast as possible. Therefore, it is very important to obtain the knowledge about the mechanism or characteristics of transport phenomena of these materials in MEA to design a high performance PEFC. However, these phenomena cannot be analyzed by conventional Computational Fluid Dynamics (CFD) simulations based on continuum theory because the MEA consists of gas diffusion layer (GDL), micro porous layer (MPL), catalyst layer (CL) and polymer electrolyte membrane (PEM), which have very fine structures whose size is of the order from nanometer to micrometer, and the reactant or product materials transport in the fine structures. Molecular simulation is a suitable scheme to analyze such flow phenomena. In this study we analyzed the nanoscale transport phenomena of the materials in MEA of PEFC by large scale molecular simulations, such as quantum calculation or molecular dynamics simulation. Especially, transport phenomena of proton and water in PEM, oxygen permeability or proton conductivity of ionomer in CL, and transport phenomena of water droplet in a nano pore were simulated, and the nanoscale transport characteristics were analyzed in detail to achieve the design of new concept of MEA for next generation PEFC.

## Biography

Takashi Tokuamsu has completed his PhD from the University of Tokyo and was Postdoctoral fellow in this University in one year. He moved to Institute of Fluid Science, Tohoku University as a Research Assistant in 1999, promoted to Lecturer in 2003, and Associate Professor in 2005. He is an Associate Professor of Institute of Fluid Science, Tohoku University. His research is basically on nanoscale transport phenomena and has published more than 40 papers in reputed journals and more than 100 times presentation in international conferences.

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