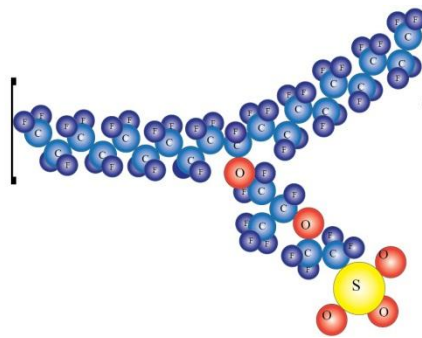


Understanding of Water and Proton Transport in Nanostructured Polymer Electrolyte Membrane using Molecular Dynamics Simulations

Mohammad Moulod

Polymer Electrolyte Membrane Fuel Cell (PEMFC) is a promising alternative clean energy source due to high energy density and efficiency with zero emission. Optimal water management is critical to the desired PEMFC performance. A key component is PEM, i.e., Nafion®, which requires hydration for good proton conductivity. In the catalyst layer, Nafion serves as a proton conductor along with the carbon and platinum nanoparticles, but the water and proton conductivity in the Nafion thin film is not fully understood. In this study, the underlying physics of the water and proton conductivity within the thin Nafion film is examined using molecular dynamic simulation. Also, with the recent emergence of the nanotechnology, graphene serves as a great potential to enhance PEMFC performance. This study will investigate the origin of the performance both experimentally and theoretically.



dry Nafion structure