



*Nanoscienze & Nanotecnologie
& Strumentazione*

Seminario

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Titolo:

**“MD simulation of Nafion[®]-related fuel-cell
membrane materials”**

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MD simulation of Nafion[®]-related fuel-cell membrane materials

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Perfluorosulphonic acid (PFSA) polymers have long been the proton-conducting membranes of choice in PEMFC and DMFC applications. Nafion[®] has indeed become the standard against which any new polymer FC membrane must be benchmarked. What then is special about this material – and how could it be improved?

Molecular Dynamics (MD) simulation can provide us with valuable insights to help answer these questions. With today's high-performance computers, simulations can be performed involving tens of thousands of atoms. I will describe MD simulations of two hydrated membrane polymers for comparison purposes: Nafion[®] and another popular FC membrane material Hyflon[®] - earlier known as the Dow[®] membrane. These two polymers differ only in the nature of their side-chains. Subtle differences are found to result in their water-channel morphologies and in the local environments and dynamics of the hydrated protons which move in their channels. These differences can help explain the differences found in the properties of these two membranes.