MD simulation of battery and fuel-cell related polymer systems.

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Both the Li-ion (polymer) battery and the polymer-based fuel cell have become strategically important technologies in recent years, not least from an environmental viewpoint. Though both are by now relatively well established, there are still large gaps in our basic understanding of the ion transport mech-anisms involved. Research effort to improve this situation will inevitably lead to improvements in these technologies. In this context, a central issue will always be the achievement of a basic understanding of atomic-level ion transport mechanisms in the polymer-membrane materials involved. Some typical examples are:

- Ionic transport in crystalline polymer electrolytes.[1]
- The effect of side-chains on ionic transport.[2]
- Ionic conductivity enhancement through the use of "nano-fillers".[3]
- Proton transport in hydrated Nafion©.[4]

In this context, the computational power of today's supercomputers is so great that Molecular Dynamics (MD) simulation can now provide valuable insights, especially into phenomena which are difficult – not to say impossible – to access experimentally. Some illustrative examples will be taken from recent work.

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