

# **Proton Transport in Biological Systems by Large-scale Car-Parrinello Simulations**

*Paolo Carloni*

*German Research School and Institute for Advanced Simulation (IAS)*

*Juelich Research Center*

*Juelich, Germany*

Proton transport plays a key role for cell metabolism. The cell membrane surface is a major pathway for it. A long-standing experimentally observed puzzle is how to reconcile fast interfacial proton migration with strong binding to the membrane surface. Here I will present results from Car-Parrinello molecular dynamics (CPMD) simulations addressing this issue. I will close my talk by presenting a recent CPMD investigation on the strikingly efficient proton conduction in the gramicidin ion channel.