Ion permeability in flow batteries and fuel cells by multiphysics modelling

Large-scale energy storage is needed in stable power-grid management and the integration of renewable sources. The redox *flow battery* (FB) provides a unique combination of high efficiency and long cycle life. The key FB components are redox pairs (usually vanadium ions), electrodes and a separating polymer membrane to prevent the electrolytes to cross mix and to transfer ions. High-quality, low-cost materials are vital to achieve large-scale acceptable FBs; ion chemistry and transport are the key factors in determining the final FB performance. In this project we use multiscale simulations to provide fundamental physical insights into the ion transport in *novel, metal free, organic-inorganic aqueous FB*. Our atomistic non-equilibrium molecular-dynamics simulations deliver polymer/electrolyte/electrode interfaces and local diffusivities for large-scale Lattice-Boltzmann simulations of permeabilities and transport in *porous media*. Our project may lead to a substantial cost reduction and increased efficiency of FB by advising experiments with improved membranes and optimized electrode geometry.