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Understanding the mechanism of proton conductivity in Metal-Organic Frameworks by QENS

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Polymer electrolyte membrane fuel cells (PEMFCs) represent an appealing option as alternative clean energy systems. Currently, commercially used proton conductors are based upon acidic polymers such as Nafion with conductivity of 10–2 S/cm in presence of water and at temperatures below 80 °C. Rational design of new electrolyte materials to tackle current technical limitations is critical to increase the efficacy of PEMFCs. Recently, metal-organic frameworks (MOFs) have been considered as alternative candidates for proton conducting applications as a result of their crystallinity (allowing insight into the proton-conduction mechanism), modular nature, tunable pores and thermal stability.

A new phosphonate-based MOF, denoted MFM-500(Ni) was synthesised and displays proton conductivity of 4.5×10^{-4} S/cm at 98 % relative humidity and 25 °C. The intrinsic proton diffusion mechanism in MFM-500(Ni) was elucidated via a combination of X-ray diffraction and quasi-elastic neutron scattering (QENS) studies giving a remarkable contribution to knowledge in this area. It was demonstrated that proton conduction in MFM-500(Ni) is mediated by a “free diffusion inside a sphere” model, representing the first example of such a mechanism observed in a MOF.

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