Experimental report

22/03/2016

Proposal: 7-05-437 **Council:** 10/2014

Title: Proton conduction in metal-organicframeworks

Research area: Chemistry

This proposal is a new proposal

Main proposer: Herve JOBIC

Experimental team: Herve JOBIC

Local contacts: Jacques OLLIVIER

Samples: MgO6(C7D4O5).2H2O
MIL-91 : AlOH(H2L).3H2O , with L=(PO3-CD2-NDC4D10-ND-CD2-PO3)

Instrument	Requested days	Allocated days	From	To
IN5	4	4	18/06/2015	22/06/2015

Abstract:

A series of phosphonate and gallate based MOFs have been recently synthesized and it has been found that these porous materials have a high conductivity. The characterization of the elementary steps associated with the mobility of protons in such systems is particularly challenging. QENS would allow us to access to the proton mobility inside the pores, in combination with molecular simulations.

Proton Transport in a Highly Conductive Porous Zirconium-Based Metal–Organic Framework: Molecular Insight

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Abstract: The water stable UiO-66(Zr)-(CO2H)2 MOF exhibits a superprotonic conductivity of 2.3×10^{-3} Scm^{-1} at 90°C and 95% relative humidity. Quasi-elastic neutron scattering measurements combined with aMS-EVB3 molecular dynamics simulations were able to probe individually the dynamics of both confined protons and water molecules and to further reveal that the proton transport is assisted by the formation of a hydrogen-bonded water network that spans from the tetrahedral to the octahedral cages of this MOF. This is the first joint experimental/modeling study that unambiguously elucidates the proton-conduction mechanism at the molecular level in a highly conductive MOF.