

Proton Conductors based on Metal Phosphonate Hybrid Materials for PEM Fuel Cells

A. Cabeza^{a,*}, R.M.P. Colodrero^a, M. Bazaga-García^a, D. Hernández Alonso^b, J.M. Compañá Prieto^a, P. Olivera-Pastor^a, E.R. Losilla^a, M.A.G. Aranda^{a,c}, L. León-Reina^d.

^a Dpto Química Inorgánica, Campus de Teatinos s/n, Universidad de Málaga, Málaga, 29071, (Spain)

^b ICIQ, Tarragona (Spain).

^c Cell ALBA Synchrotron radiation facility, Ctra. BP1413 km 3.3, 08290 Cerdanyola del Vallès, Barcelona, (Spain).

^d Servicios Centrales de Apoyo a la Investigación, SCAI, Universidad de Málaga, Campus Teatinos s/n. 29071-Málaga (Spain)

*Corresponding author: aurelio@uma.es

Summary

The necessity of energy and power generation is constantly growing. Fossils fuels are quickly becoming unsatisfactory substrates due to both their emission of pollutants and their finite expectancy. Fuel cells are one of the best alternatives as they are clean, durable, and highly efficient¹. MOFs will be attractive candidates for this application because of their tuneable pore size functionality as well as their chemical and thermal stability and presence of acidic protons within their structure².

In the present work, we report the syntheses, crystal structural and proton conductivities of various metal phosphonate derivatives, using both rigid (5-(dihydroxyphosphoryl)isophthalic acid, PiPhtA and 2-hydroxyphosphonoacetic acid, HPAA) and flexible (hexa- or octamethylenediamine-N,N,N',N'-tetrakis-(methylenephosphonic acid, H₆HDTMP or H₈ODTMP) multifunctional ligands. These materials show 3D open-frameworks containing 1D channels decorated with phosphonic and carboxylic acid groups and filled with hydrogen bonded water molecules what make them good candidates as proton conductors. For instance, Ca-PiPhtA, containing a rigid ligand, exhibits a proton conductivity of $5.7 \cdot 10^{-4}$ S/cm which increases to $6.6 \cdot 10^{-3}$ S/cm when the sample is exposed to ammonia vapors³. Other magnesium or lanthanides metal phosphonates, built with flexible ligands, show conductivities values range between $1.6 \cdot 10^{-3}$ S/cm (for MgODTMP⁴) and $8.6 \cdot 10^{-3}$ S/cm (for LaHDTMP⁵) at T=292K at ~100% relative humidity, and activation energies values typically attributed to a Grotthuss mechanism.

Keywords: Fuel Cells, MOFs, Proton conductivity, Metal Phosphonates, Grotthuss Mechanism.

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