Experimental report

15/07/2021

Proposal: **EASY-642** **Council:** 4/2020

Title: Confined water in Benzene Mesoporous Organosilica

Research area: Materials

This proposal is a new proposal

Main proposer: **Mirian CASCO**

Experimental team:

Local contacts: Monica JIMENEZ RUIZ

Samples: Mesoporous organic silica

Instrument	Requested days	Allocated days	From	To
IN1	24	24	19/08/2020	20/08/2020

Abstract:

In recent studies, we have shown that the physical properties of confined water, such as mobility and phase state, has a tremendous impact on the water-to-hydrate conversion in ordered mesoporous carbons[1]. Silica, however, is the basic component of rock where most hydrate is found. Therefore, we aim to study by INS the impact of silica polarity on the phase properties of confined water. To this end, we selected benzene mesoporous organosilica (BMO) because it is a model material that combines highly ordered pore structure with well-defined surface chemistry within cylindrical pores offering an ideal scenario to investigate confined fluids[2]. The water partially wets BMO due to the alternation between silanol and benzene groups on its surface[3]. This special feature dramatically changes the water behavior comparing to the well-known MCM-41 that exhibits merely silanol groups (uniform wetting). Therefore, we propose to measure in Lagrange: dry BMO and BMO loaded with water. Two water content will be carefully selected in order to ensure that water is in mesopores. [1] J. Phys. Chem. C, 2019, 123, 24071, [2]Langmuir, 2013, 29, 14893, [3]Angew. Chemie - Int. Ed., 2017, 56, 12348

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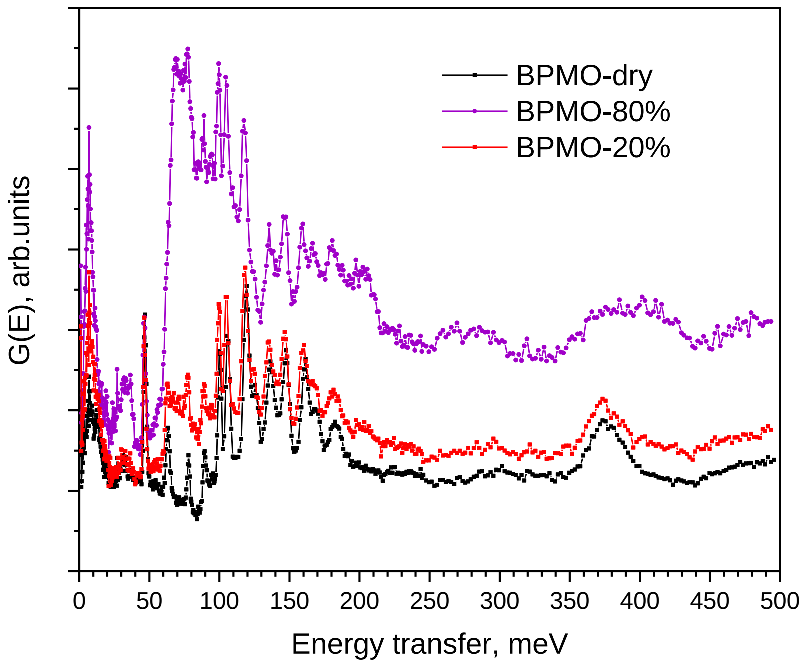
Report

In recent studies, we have shown that the physical properties of confined water, such as mobility and phase state, has a tremendous impact on the water-to- hydrate conversion in ordered mesoporous carbons[1]. Silica, however, is the basic component of rock where most hydrate is found. Therefore, we aim to study by inelastic neutron scattering the impact of silica polarity on the phase properties of confined water. To this end, we selected benzene mesoporous organosilica (BPMO) because it is a model material that combines highly ordered pore structure with well-defined surface chemistry within cylindrical pores offering an ideal scenario to investigate confined fluids.[2] The water partially wets BPMO due to the alternation between silanol and benzene groups on its surface. This special feature dramatically changes the water behavior comparing to the well-known MCM-41 that exhibits merely silanol groups (uniform wetting). Therefore, we have proposed to measure in Lagrange: dry BPMO and BPMO loaded with water. Two water content were carefully selected in order to ensure that water is in mesopores, then 20 and 80% of total pore volume were loading with water, BPMO-20 and BPMO-80, respectively.

The INS spectra results are shown in **Figure 1**, they were measured with a resolution in energy of 2% Ei. The data for dry BPMO and BPMO-20 are normalized to the mass. The peak at about 46 meV showed the same intensity in the spectra for both sample, therefore, sample BPMO-80 was normalized to this peak. (not published data)



[1]M. E. Casco, et al. *J. Phys. Chem. C*, 2019, **123**, 24071–24079. [2]M.Thommes, et al. *Langmuir*, 2013, **29**, 14893–14902. [3]J. B. Mietner, et al. *Angew. Chemie - Int. Ed.*, 2017, **56**, 12348–12351.