Experimental Report

17/01/2014

Proposal: **DIR-105** **Council:** 10/2012

Title: Tests of carbon structures models using diffusion data

This proposal is a new proposal

Researh Area:

Main proposer: **JOBIC HERVE**

Experimental Team: JOBIC HERVE

Local Contact: OLLIVIER Jacques

Samples: Carbons: C
Adsorbates: CH4, CF4, CCL4, C(CH3)4, H2

Instrument	Req. Days	All. Days	From	To
IN6	7	7	21/02/2013	28/02/2013

Abstract:

The diffusion of H_2 and CH_4 in two zeolite template carbons (ZTC) was successfully studied on IN6. Some typical spectra obtained in FAU-ZTC are shown on Figure 1. A complication occurs because of the variation of the small-angle scattering from the carbon upon adsorption, resulting in a negative elastic contribution; nevertheless, the spectra can be fitted and a variation of the broadening, hence of the diffusivity, is put into evidence with the loading: it presents a maximum at intermediate methane concentration. Comparisons are now being made with molecular simulations for the derived self-diffusion coefficients.

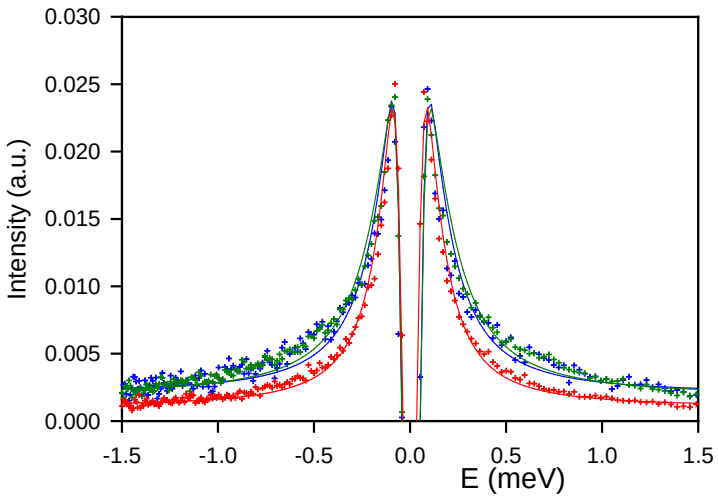

Figure 1. Comparison between experimental and simulated spectra for methane adsorbed at different loadings in FAU-ZTC : θ_1 (in blue), θ_3 (in green), θ_4 (in red), (Q = 0.32 Å^{-1}, T = 250 K).

During the allocated beam time, the diffusion of gases with different kinetic diameters was studied as a function of temperature in a carbide-derived carbon (CDC). The diffusivities were derived for a low sorbate concentration and activation energies for diffusion could be obtained for the different gases: methane, cyclopropane, sulfur hexafluoride, and neopentane. Simulations are in progress to obtain comparable data.