Understanding Methane Adsorption in Porous Aromatic Frameworks: An FTIR, Raman, and Theoretical Combined Study

M. Errahali, G. Gatti, L. Tei, L. Canti, A. Fraccarollo, M. Cossi, L. Marchese*

Dipartimento di Scienze e Innovazione Tecnologica and Centro Nano-SiSTeMI, Università del Piemonte Orientale "A. Avogadro", Via T. Michel 11 - 15121 Alessandria, Italy

***Corresponding author:** leonardo.marchese@mfn.unipmn.it

1. Solid-state ^{13}C MAS NMR
2. Powder XRD
3. TGA curve
5. SEM
6. GCMC adsorption isotherms of CH_4 on PAF-302
7. IR difference spectra of CD_4 adsorbed on PAF-302

Solid-state ^{13}C MAS NMR

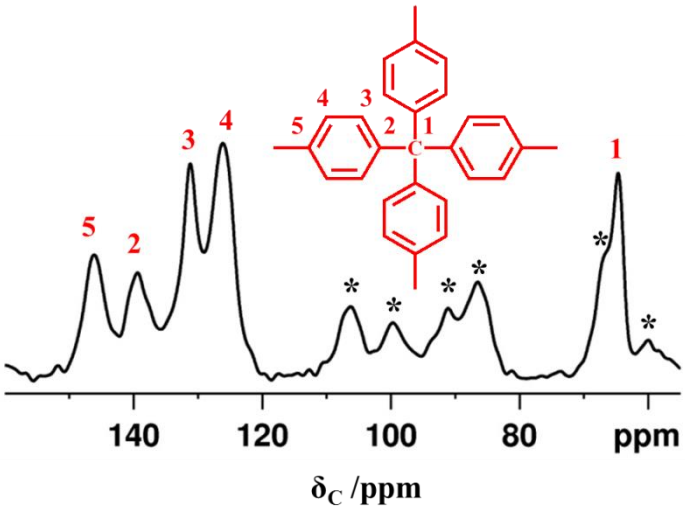

Figure S1 : ^{13}C solid state CPMAS NMR spectra of PAF302. A cross polarization contact time of 5 ms and a MAS spin rate of 5 kHz were used in the experiment. * denotes spinning sidebands.

Powder XRD

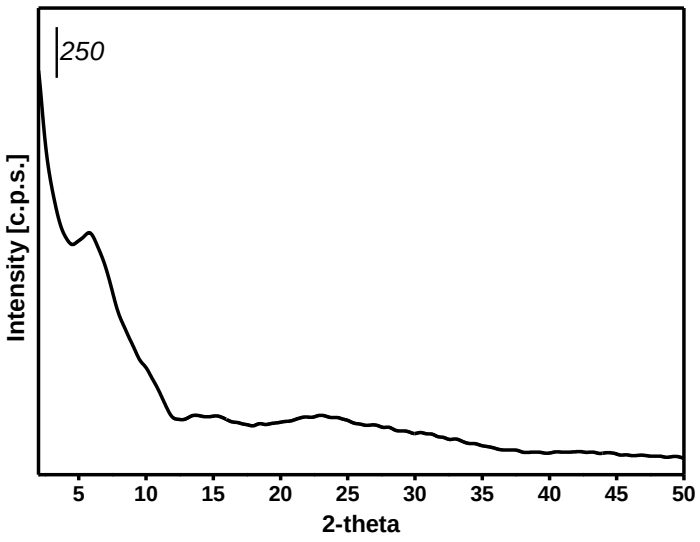

Figure S2 : Powder XRD pattern of PAF-302

Thermogravimetric analysis (TGA)

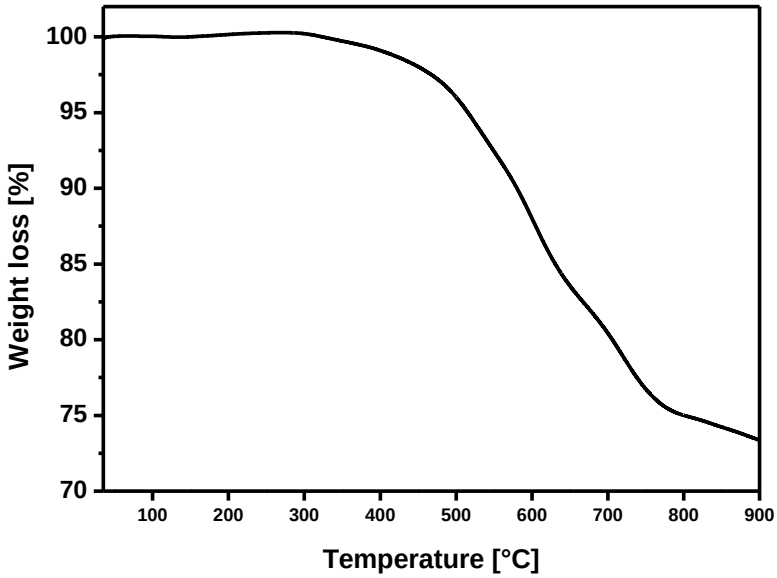

Figure S3 : Thermogram of PAF-302 under argon atmosphere

Scanning electron microscopy (SEM)

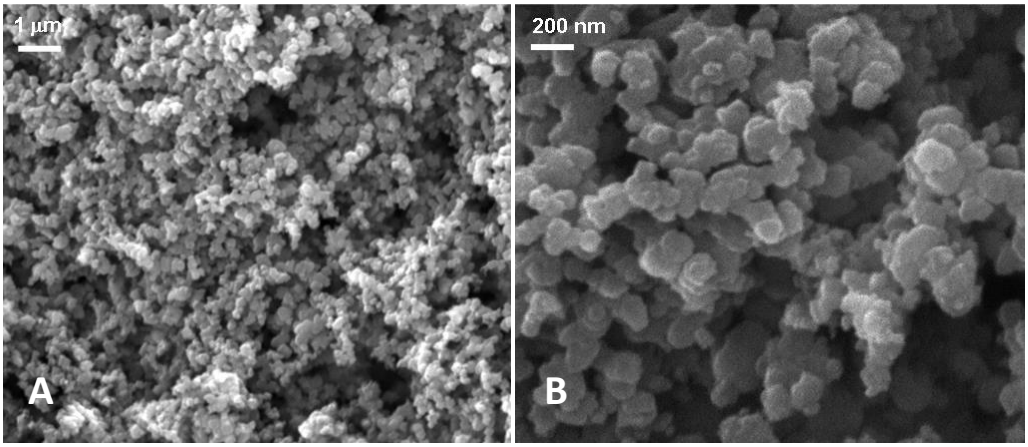

Figure S4 : SEM image of PAF-302 at 25000X A) and 100000X B)

GCMC adsorption isotherms of CH_4 on PAF-302

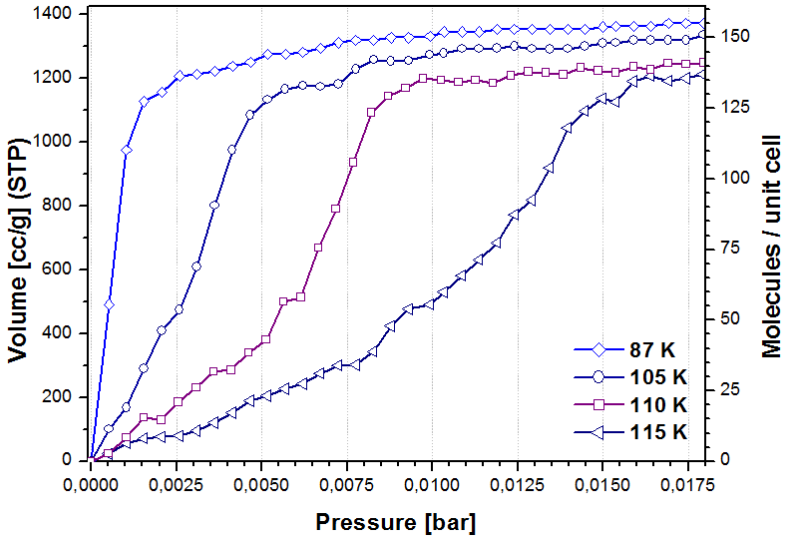

Figure S5 : Adsorption isotherms of CH_4 on PAF-302 at different temperatures: the isotherms were simulated with Grand Canonical Monte Carlo (GCMC) method using a force field specifically designed to study methane adsorption in PAF materials[19]

IR difference spectra of CD_4 adsorbed on PAF-302

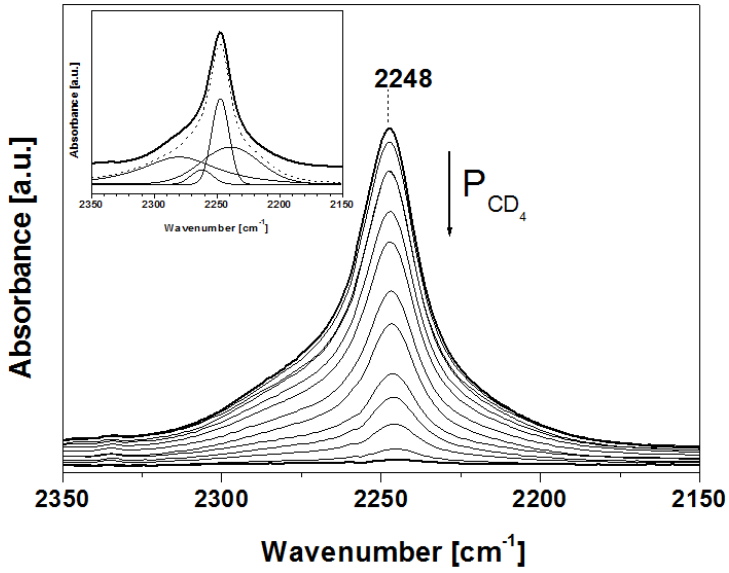

Figure S6 : IR difference spectra in the 2350-2150 cm^{-1} range of CD_4 adsorbed at 110 K at different pressures (the equilibrium pressure was varied from 8.4, the most intense curve, to 0.21 mbar); The inset shows the spectrum at the highest CD_4 loading (top solid line) fitted by four Gaussian curves. The overall spectrum obtained by adding the four components (dotted line) is reported for comparison.