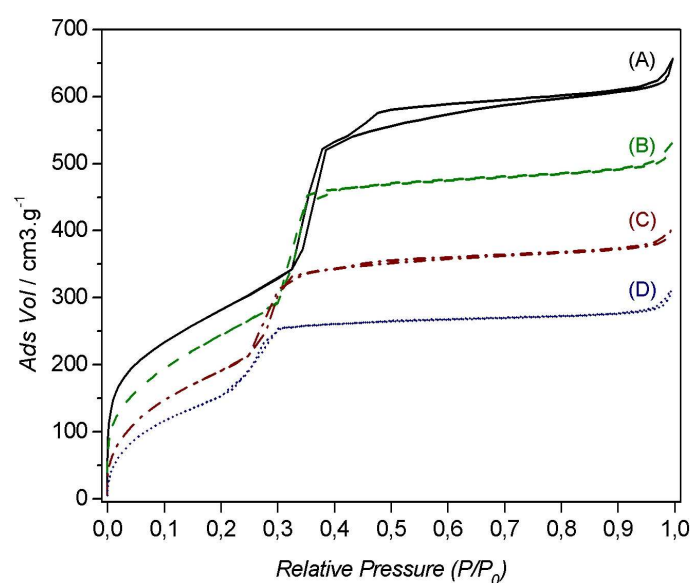


# Electronic Supplementary Information

## Design of grafted copper complex in mesoporous silica in defined coordination, hydrophobicity and confinement states

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**Fig. S1** N<sub>2</sub> sorption isotherms at 77 K of materials **1**(A), **2**(B), **3**(C) and **5a**(D).

**Table S1.** Molecular ratio deduced from XPS analysis (note that X/Si molar ratio are reported here for total silicon; when X/Si<sub>inorg</sub> is at stake, the data has to be multiplied by 1.22, 1.26 and 1.24 for **4**, **5a** and **5b**, respectively, according to the number of organic silicon shown in Table 2 as (TMS+BPS)/Si<sub>inorg</sub>).

| Sample | <b>4</b>    | <b>5a</b>   | <b>5b</b>   |
|--------|-------------|-------------|-------------|
| Br/Si  | 0.010±0.003 | 0.009±0.004 | 0.006±0.004 |
| N/Si   | 0.079±0.004 | 0.067±0.004 | 0.052±0.004 |
| Cu/Si  |             | 0.015±0.004 | 0.007±0.003 |
| Cl/Si  |             | 0.019±0.003 |             |
| F/Si   |             |             | 0.025±0.004 |
| F/Cu   |             |             | 3.4±0.5     |
| Cl/Cu  |             | 1.3±0.6     |             |
| Br/Cu  |             | 0.6±0.4     | 0.4±0.2     |
| N/Cu   |             | 4.5±1.4     | 7±3         |

**Table S2.** XPS data for grafted materials **4**, **5a** and **5b**. Binding energy in eV and the percentage obtained from deconvolution in parenthesis.

| Material           | 4                | 5a               | 5b               |
|--------------------|------------------|------------------|------------------|
| <b>Br (3d) /eV</b> | 68.2<br>(32.1%)  | 68.5<br>(25.9%)  | 68.4<br>(23.6%)  |
|                    | 70.6<br>(67.9%)  | 70.7<br>(74.1%)  | 70.5<br>(76.4%)  |
| <b>N (1s) /eV</b>  | 399.9<br>(85.7%) | 399.6<br>(90.6%) | 399.7<br>(90.7%) |
|                    | 401.7<br>(14.3%) | 401.7<br>(9.4%)  | 402.0<br>(9.3%)  |

**Table S3.** EXAFS fit quality criteria.

| Samples   | Fit quality criteria                                                    |
|-----------|-------------------------------------------------------------------------|
| <b>6a</b> | QF = 0.82<br>( $\rho$ =0.4%)<br>$\nu$ = 4<br>$\Delta E_0 = 6.2 \pm 0.3$ |
| <b>5a</b> | QF = 0.90<br>( $\rho$ =1.8%)<br>$\nu$ = 8<br>$\Delta E_0 = 1.8 \pm 0.7$ |
| <b>6b</b> | QF = 1,04<br>( $\rho$ =0.6%)<br>$\nu$ = 5<br>$\Delta E_0 = 3.3 \pm 0.8$ |
| <b>5b</b> | QF = 1,00<br>( $\rho$ =1.7%)<br>$\nu$ = 6<br>$\Delta E_0 = 1,8 \pm 0.8$ |