Supramolecular assembly of methyl-substituted cucurbit[6]uril and

potential applications in selective sorption

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EXPERIMENTAL SECTION

Experimental details on the sorption/desorption

1. Activation

We have activated the crystalline material by heating up to 80°C (0.08Mpa, 4h) before sorption measurements. Meanwhile, we have activated the HMeQ[6] powder in the same conditions.

2. Sorption

We placed the activated samples and volatile material in a sealed bottle (as shown below). And then weighed two samples each certain time interval quickly, until the weight didn't change.



3. Desorption

We deal the samples by heating up to 80°C (0.08Mpa, 4h).



Figure S1 The sorption isotherms of Methanol at 298 K. \blacksquare symbol = adsorption and, \star symbol = desorption of the HMeQ[6] -based porous material and HMeQ[6] powder respectively.



Figure S2 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for methanol.



Figure S3 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for ethanol.



Figure S4 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for acetone.



Figure S5 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for acetonitrile.



Figure S6 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for tetrachloromethane.



Figure S7 Volatile materials sorption profiles of (■) the HMeQ[6]-based porous material, and (●) HMeQ[6] powder for diethyl ether.



Figure S8 Volatile materials sorption profiles of (**•**) the HMeQ[6]-based porous material, and (**•**) HMeQ[6] powder for dichloromethane.



Figure S9 Recyclability tests for methanol adsorption of the HMeQ[6]-based porous material and HMeQ[6] powder.



Figure S10 Powder X-ray diffraction (PXRD) of the HMeQ[6]-based porous material and the corresponding comparison with simulation.



Figure S11 DSC (a) and TG (b) curves of the HMeQ[6]-based porous material and the corresponding comparison with HMeQ[6] powder, hydroquinone powder in N_2 .