



## SUPPORTING INFORMATION

## Influence of silicodactyly in the preparation of hybrid

## materials

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**Figure S1**The XRD pattern of plain MCM-41 (curve a ), MeO-MCM-41 (curve b), diMeO-MCM-41 (curve c) and triMeO-MCM-41 (curve d).



Figure S2. TGA curves of plain MCM-41 (a), MeO-MCM-41(b), diMeO-MCM-41 (c) and triMeO-MCM-41 (d).



Figure S3. DTG curves of plain MCM-41 (black), MeO-MCM-41 (red), diMeO-MCM-41 (green) and triMeO-MCM-41 (blue).



**Figure S4.** The simulation box contains one mercapto-propyl alkoxysilane derivative grafted on slab silica and periodic boundary conditions in all direction are used.