

Supplementary Information

Au nanoparticles encapsulated into Al-MCM-41 mesoporous material: In-situ synthesis and electronic structure

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Table S1 The textural characteristics of the samples

Sample	d_{110} / nm	a_0 / nm	S_{BET} / $\text{m}^2 \cdot \text{g}^{-1}$	V / $\text{mL} \cdot \text{g}^{-1}$	D_{BJH} / nm	t / nm
Al-MCM-41	3.93	4.54	873.6	0.97	3.94	0.47
Au/Al-MCM-41	3.82	4.41	706.5	0.50	3.69	0.85

a_0 -pore parameter ($=2d_{100}/\sqrt{3}$), t -pore wall thickness ($t=a_0-D_{\text{BJH}}$), V -pore volume

Table S2 The element concentrations in the leaching solution (from ICP analysis, with pH adjusted to 8).

The concentration of Al is estimated from XPS analysis of the calcined sample Al-MCM-41, with the concentration of Si taken as reference. The actual concentrations are highlighted in bold.

Elements	Concentrations in leaching solution from ICP at pH 8 (ug/mL)	Estimated concentrations from XPS (ug/mL)
Al	0.12	2.78
Fe	0.03	/
Mg	0.23	/
K	28.5	/
Na	>1500	/
Si	275.4	275.4

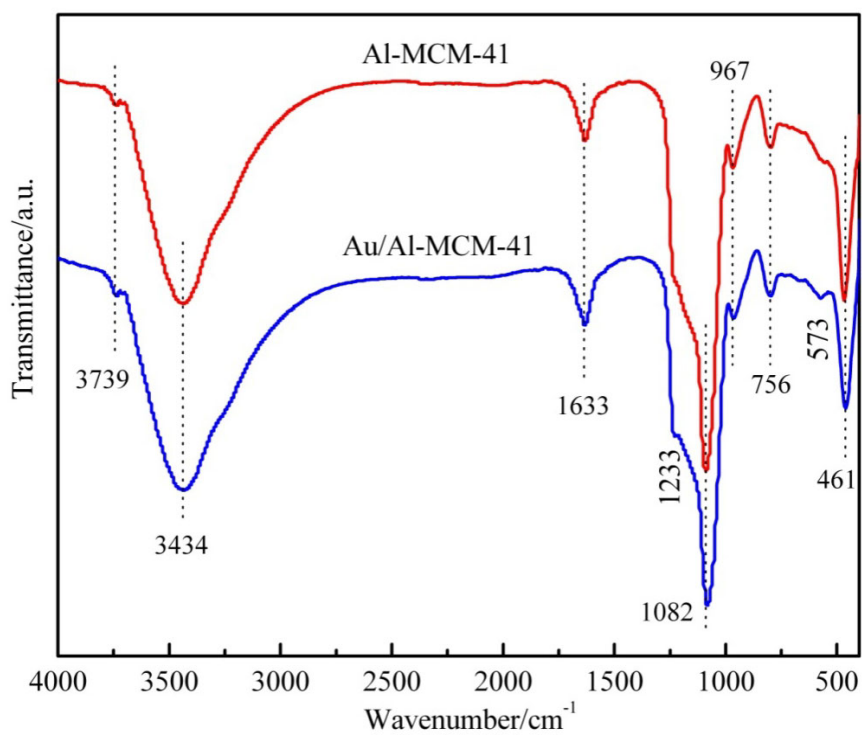


Fig. S1 FTIR spectra of different samples.

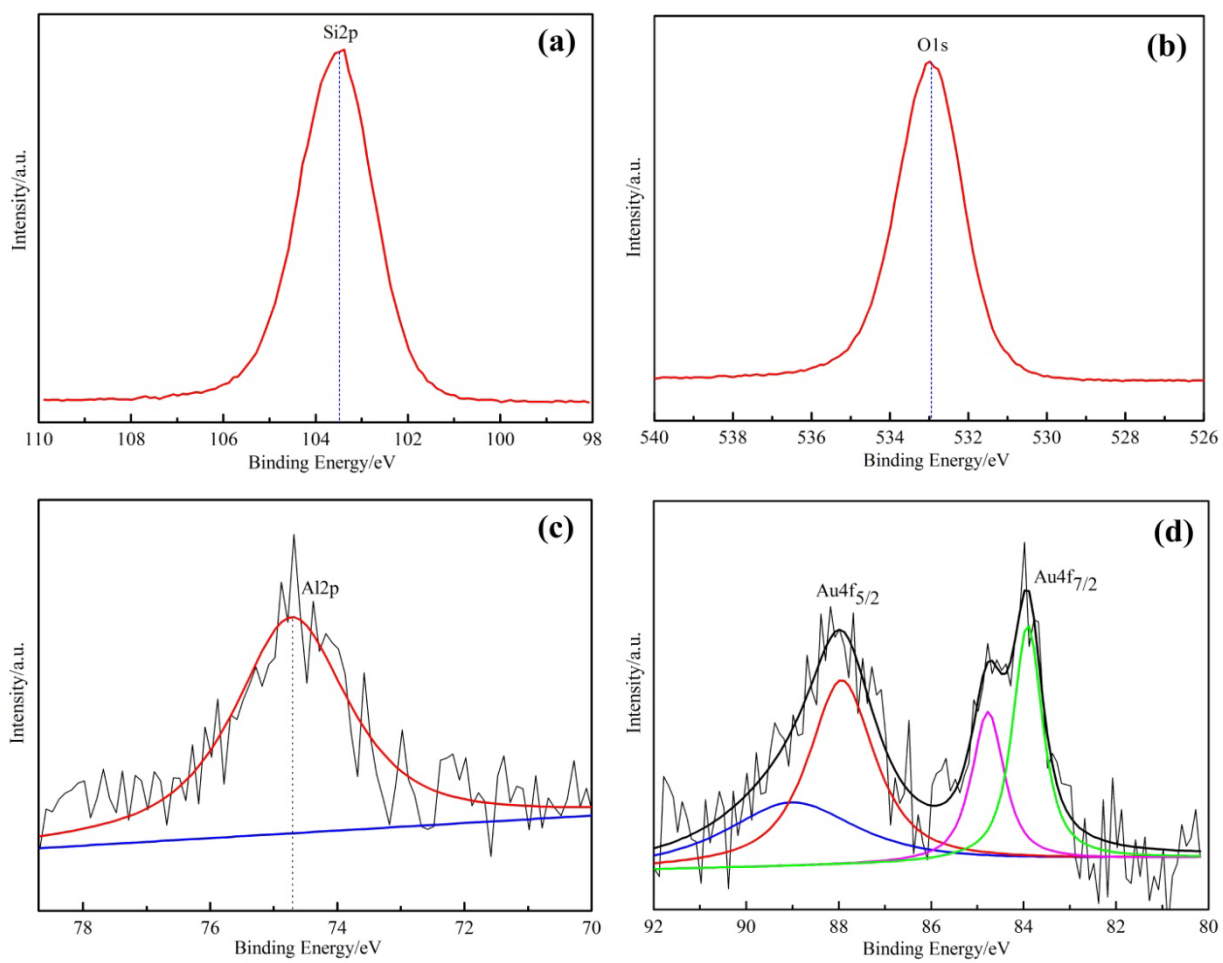


Fig. S2 (a) Si2p, (b) O1s, (c) Al2p, and (d) Au4f XPS spectra of Au/Al-MCM-41.

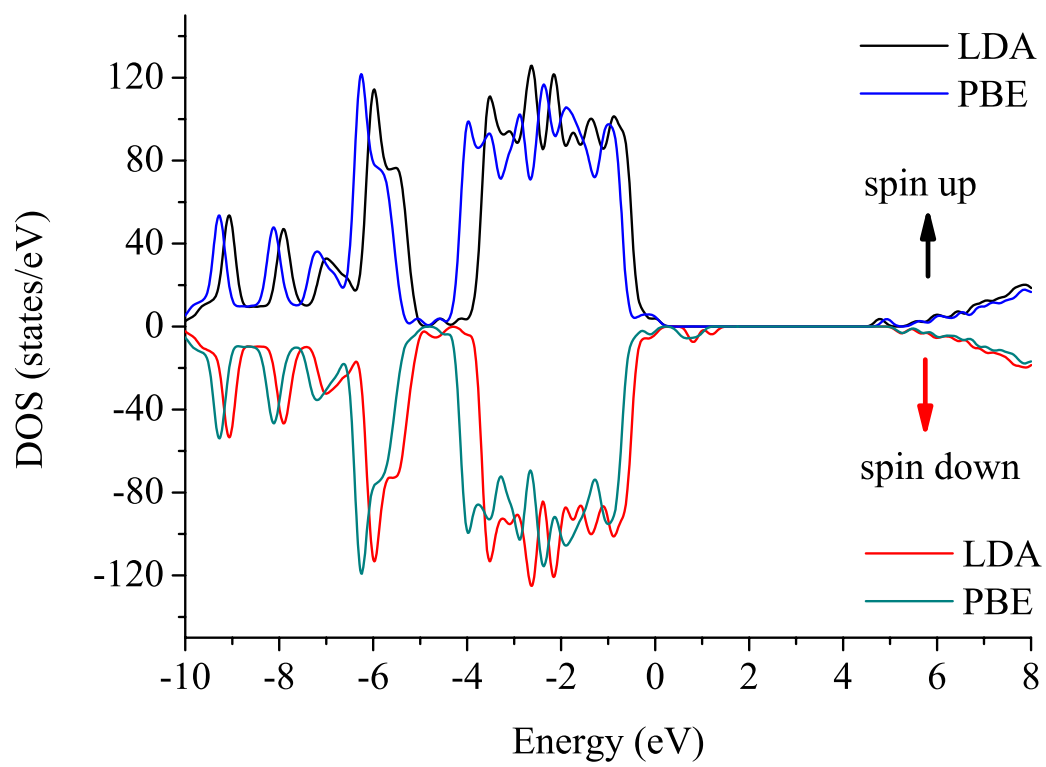


Fig. S3 The spin-polarized total density of states (DOS) for Au doped silica. Both LDA and PBE results are given.