Supporting Information

An ultrastable La-MOF for catalytic hydrogen transfer of furfural: in-situ activation of surface

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Computational Method.

All density functional theory calculations were performed using the Vienna ab initio simulation package (VASP). [1, 2] The generalized gradient approximation of Perdew–Burke–Ernzerhof (PBE) was emplyeded to describe the exchange-correlation.[3] The cut-off energy of 400 eV was used for the plane wave, and the ionic positions of all structures were relaxed until the force converged to below -0.05 eV·Å^{-1}. A k-point of 2 × 2 × 3 set was adopted. The vacuum space between slabs along the *z*-direction was set at a minimum of 15 Å. Moreover, charges transfer are analyzed based on the Bader theory.[4]

[1] Kresse, G.; Furthmüller, J. Comput. *Mater. Sci*. 1996, 6, 15−50.

[2] Kresse, G.; Furthmüller, J. Phys. Rev. B: Condens. *Matter Mater. Phys*. 1996, 54, 11169−11186.

[3] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. *Rev. Lett.* 77 (1996) 3865–3868.

[4] R.F.W. Bader, Atoms in Molecules: A Quantum Theory, International Series of Monographs on Chemistry, Clarendon Press, Oxford, 1990.

Fig. S1 Coordination environment diagram of La_1 and La_2 in LaQS

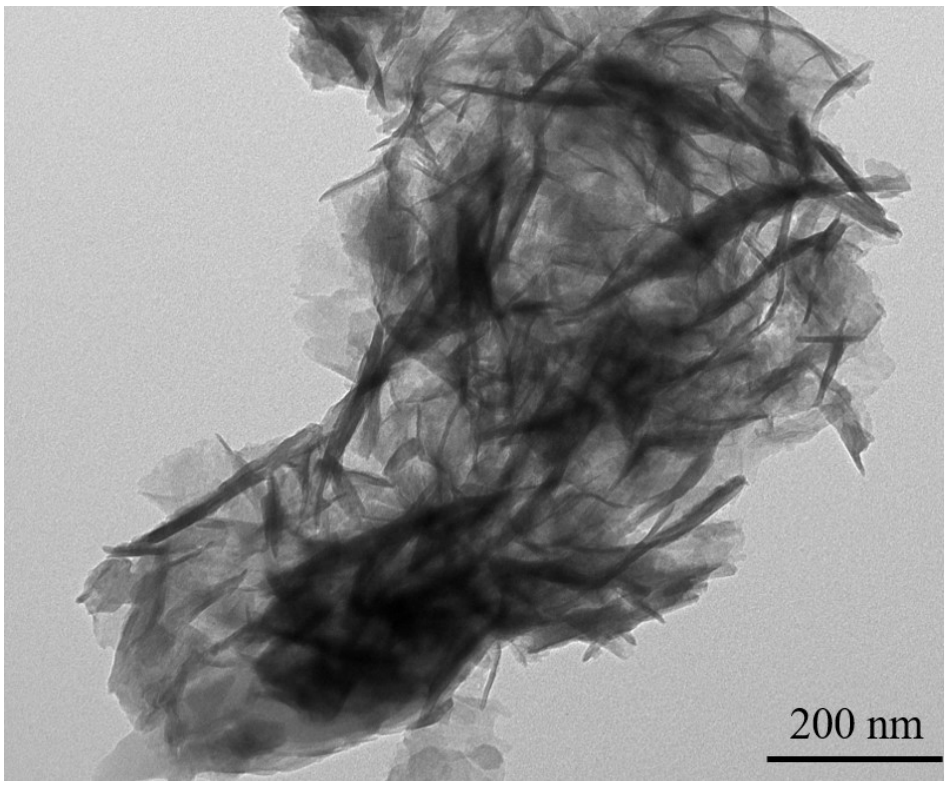

Fig. S2. TEM of LaQS lamellar structure

Table S1. Different N contents in LaQS and LaQS-A

Sample	$N_{Quinoline}$ (%)	N_{DMF} (%)
LaQS	31.00	65.48
LaQS-A_1	63.3	34.63
LaQS-A_2	68.37	28.78
LaQS-A_3	74.14	24.46

Table S2. Specific surface area, pore volume, pore size of LaQS and LaQS-A

Sample	$S_{Langmuir}$	Pore Volume (cm^3g^{-1})	Pore Size (nm)
LaQS	293.24	0.14	3.61
LaQS-A_1	621.74	0.31	3.57
LaQS-A_2	827.77	0.36	2.64
LaQS-A_3	843.37	0.34	2.50

Table S3. Selected Bond Lengths (Å) and Selected Bond Angles (deg) for the compound of LaQS

La(1)-O(3)#1	2.547(5)	La(1)-O(3)#2	2.547(5)
La(1)-O(3)	2.547(5)	La(1)-O(1)	2.550(5)
La(1)-O(1)#2	2.550(5)	La(1)-O(1)#1	2.550(5)
La(1)-O11#2	2.598(6)	La(1)-O(5)#2	2.598(6)
La(1)-O(5)#1	2.598(6)	La(1)-O11#1	2.598(6)
La(1)-O11	2.598(6)	La(1)-O(5)	2.598(6)
La(2)-O(1)	2.508(5)	La(2)-O(1)#2	2.508(5)
La(2)-O(1)#1	2.508(5)	La(2)-O(2)#1	2.516(5)
La(2)-O(2)#2	2.516(5)	La(2)-O(2)	2.516(5)
La(2)-N(1)#1	2.801(6)	La(2)-N(1)	2.802(6)
La(2)-N(1)#2	2.802(6)		
O(3)#1-La(1)-O(3)#2	74.75(19)	O(3)#1-La(1)-O(3)	74.75(19)
O(3)#2-La(1)-O(3)	74.75(19)	O(3)#1-La(1)-O(1)	144.99(15)
O(3)#2-La(1)-O(1)	96.23(16)	O(3)-La(1)-O(1)	136.42(15)
O(3)#1-La(1)-O(1)#2	96.23(16)	O(3)#2-La(1)-O(1)#2	136.42(15)
O(3)-La(1)-O(1)#2	144.99(15)	O(1)-La(1)-O(1)#2	66.78(16)
O(3)#1-La(1)-O(1)#1	136.42(15)	O(3)#2-La(1)-O(1)#1	144.99(15)
O(3)-La(1)-O(1)#1	96.23(16)	O(1)-La(1)-O(1)#1	66.78(16)
O(1)#2-La(1)-O(1)#1	66.79(16)	O(3)#1-La(1)-O11#2	71.13(18)
O(3)#2-La(1)-O11#2	67.25(18)	O(3)-La(1)-O11#2	134.01(18)
O(1)-La(1)-O11#2	74.19(17)	O(1)#2-La(1)-O11#2	69.49(16)
O(1)#1-La(1)-O11#2	129.75(16)	O(3)#1-La(1)-O(5)#2	71.13(18)
O(3)#2-La(1)-O(5)#2	67.25(18)	O(3)-La(1)-O(5)#2	134.01(18)
O(1)-La(1)-O(5)#2	74.19(17)	O(1)#2-La(1)-O(5)#2	69.49(16)
O(1)#1-La(1)-O(5)#2	129.75(16)	O(3)#1-La(1)-O(5)#1	67.24(18)
O(3)#2-La(1)-O(5)#1	134.01(18)	O(3)-La(1)-O(5)#1	71.12(18)
O(1)-La(1)-O(5)#1	129.75(16)	O(1)#2-La(1)-O(5)#1	74.19(17)
O(1)#1-La(1)-O(5)#1	69.49(17)	O(5)#2-La(1)-O(5)#1	119.995(5)
O(3)#1-La(1)-O11#1	67.24(18)	O(3)#2-La(1)-O11#1	134.01(18)
O(3)-La(1)-O11#1	71.12(18)	O(1)-La(1)-O11#1	129.75(16)
O(1)#2-La(1)-O11#1	74.19(17)	O11#2-La(1)-O11#1	119.995(5)
O(1)#1-La(1)-O11#1	69.49(17)	O(3)#1-La(1)-O11	134.01(18)
O(3)#2-La(1)-O11	71.12(18)	O(1)-La(1)-O11	69.49(17)
O(3)-La(1)-O11	67.24(18)	O(1)#2-La(1)-O11	129.75(16)
O(1)#1-La(1)-O11	74.19(17)	O11#1-La(1)-O11	119.994(3)
O11#2-La(1)-O11	119.996(5)	O(3)#1-La(1)-O(5)	134.01(18)
O(3)#2-La(1)-O(5)	71.12(18)	O(1)-La(1)-O(5)	69.49(17)

O(3)-La(1)-O(5)	67.24(18)	O(1)#2-La(1)-O(5)	129.75(16)
O(1)#1-La(1)-O(5)	74.19(17)	O(5)#1-La(1)-O(5)	119.994(3)
O(5)#2-La(1)-O(5)	119.996(5)	O(1)-La(2)-O(1)#2	68.04(17)
O(1)-La(2)-O(1)#1	68.04(17)	O(1)-La(2)-O(2)#1	131.16(15)
O(1)#2-La(2)-O(1)#1	68.04(17)	O(1)#2-La(2)-O(2)#1	93.39(16)
O(1)#1-La(2)-O(2)#1	147.42(15)	O(1)#2-La(2)-O(2)#2	147.42(15)
O(1)-La(2)-O(2)#2	93.39(16)	O(1)#1-La(2)-O(2)#2	131.16(15)
O(2)#1-La(2)-O(2)#2	78.69(19)	O(1)#2-La(2)-O(2)	131.16(15)
O(1)-La(2)-O(2)	147.42(15)	O(1)#1-La(2)-O(2)	93.39(16)
O(2)#1-La(2)-O(2)	78.69(19)	O(1)-La(2)-N(1)#1	79.05(16)
O(2)#2-La(2)-O(2)	78.69(19)	O(1)#2-La(2)-N(1)#1	126.22(16)
O(1)#1-La(2)-N(1)#1	60.49(15)	O(2)#2-La(2)-N(1)#1	72.04(17)
O(2)#1-La(2)-N(1)#1	139.29(17)	O(2)-La(2)-N(1)#1	68.42(17)
O(1)-La(2)-N(1)	60.49(15)	O(1)#1-La(2)-N(1)	126.22(16)
O(1)#2-La(2)-N(1)	79.05(16)	O(2)#1-La(2)-N(1)	72.04(17)
O(2)#2-La(2)-N(1)	68.42(17)	N(1)#1-La(2)-N(1)	119.840(17)
O(2)-La(2)-N(1)	139.29(17)	O(1)#1-La(2)-N(1)#2	79.05(16)
O(1)-La(2)-N(1)#2	126.21(16)	O(2)#1-La(2)-N(1)#2	68.42(17)
O(1)#2-La(2)-N(1)#2	60.48(15)	O(2)#2-La(2)-N(1)#2	139.29(17)
O(2)-La(2)-N(1)#2	72.04(17)	N(1)-La(2)-N(1)#2	119.840(17)
N(1)#1-La(2)-N(1)#2	119.843(17)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+y+1,-x+1,z #2 -y+1, x-y, z #3 x, y, z+1

#4 x, y, z-1 #5 y, -x+y, -z+1 #6 x-y, x, -z+1