Supplementary Information

High Hydrogen Release Catalytic Activity by Quasi-MOF Prepared via Post-Synthetic Pore Engineering

Minoo Bagheri^a, Mohammad Yaser Masoomi^{a*}, Esther Domínguez,^b and Hermenegildo García^{b*}

^{*a*} Department of Chemistry, Faculty of Science, Arak University, Arak 38156-8-8349, Iran Email: <u>m-masoomi@araku.ac.ir</u>

b Instituto Universitario de Tecnología Química, Universitat Politecnica de Valencia-Consejo Superor de Investigaciones Científicas, Av. De los Naranjos s/n, 46022 Valencia, Spain. E-mail: <u>hgarcia@upv.es</u>

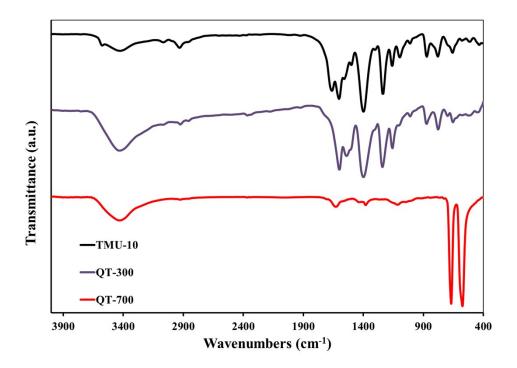


Figure S1. IR spectra of TMU-10 and QT-x samples.

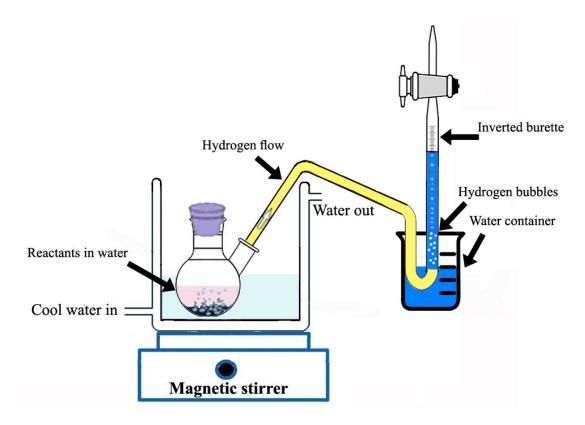


Figure S2. Schematic representation of hydrogen generation reaction setup.

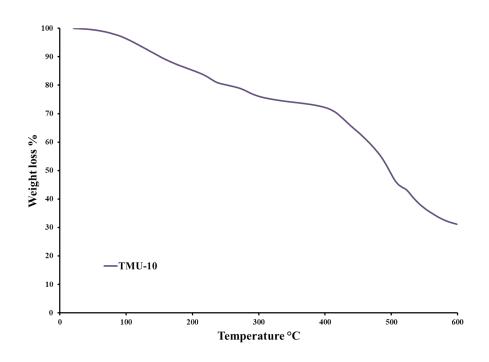


Figure S3. Thermogravimetric profiles of TMU-10.

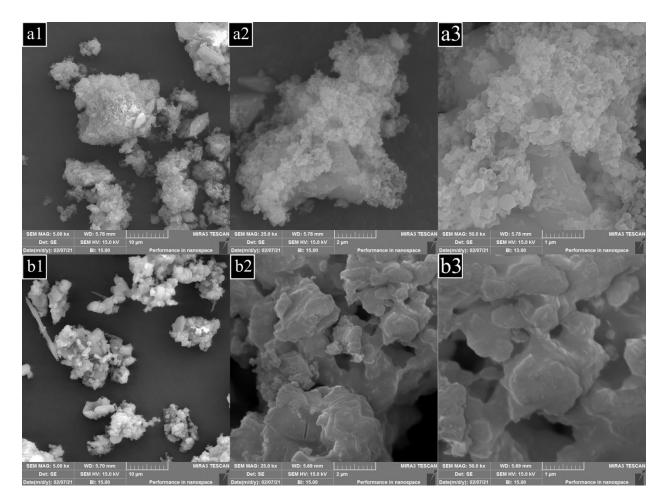


Figure S4. FE-SEM images of TMU-10 (a) and QT-300 (b) samples.

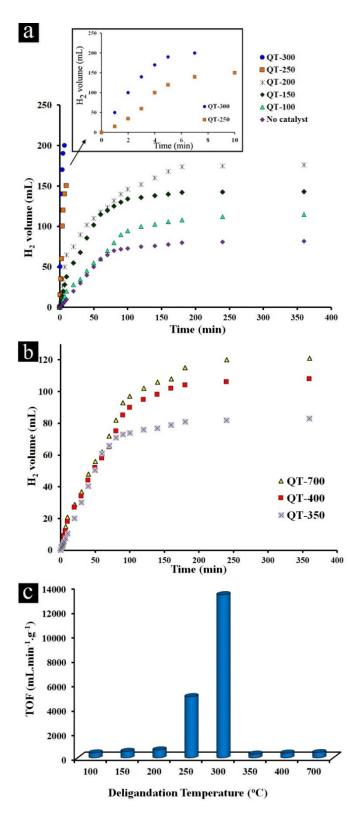


Figure S5. Time plots of the hydrolysis of NaBH₄ catalyzed by various QT-x samples at different deligandation temperatures (a, b). Comparison of TOF values related to various QT-x catalysts: experimental conditions [NaBH₄] = 125 mM, catalyst dosage = 1.5 mg T= RT.

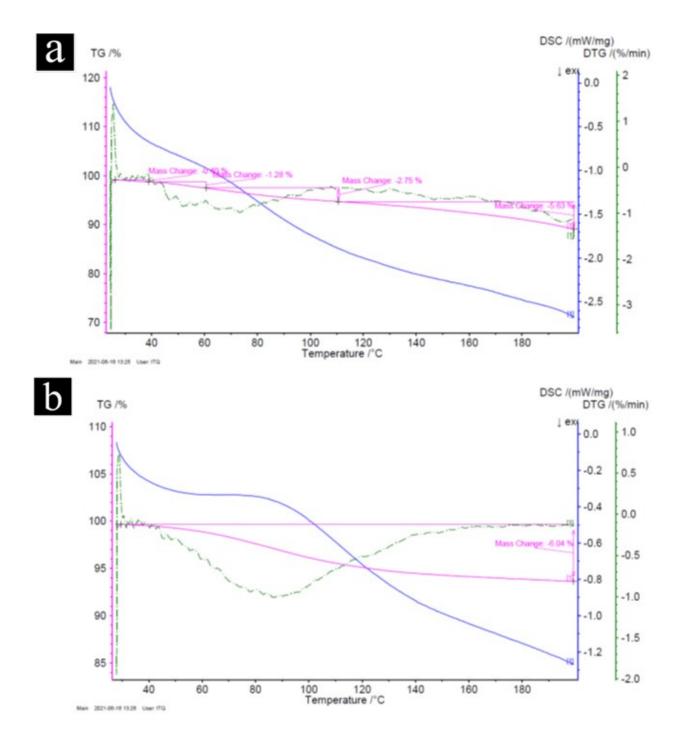


Fig. S6. Thermogravimetric analysis of ambient equilibrated (a) TMU-10 and (b) QT-300 showing their water content related to hydrophilicity.

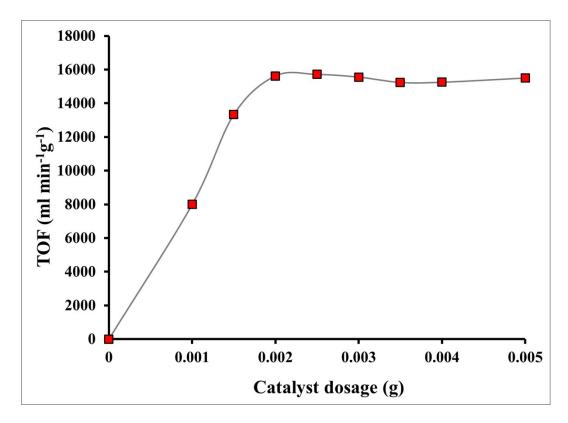


Figure S7. TOF values in presence of various amount of QT-300 catalyst.

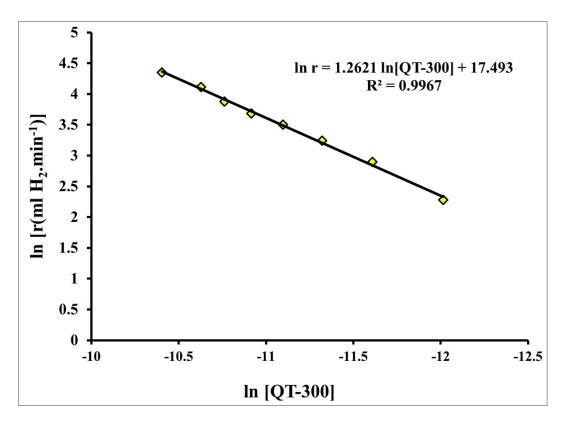


Figure S8. Plot of H_2 generation rate versus the concentration of QT-300 catalyst both in natural logarithmic scales.

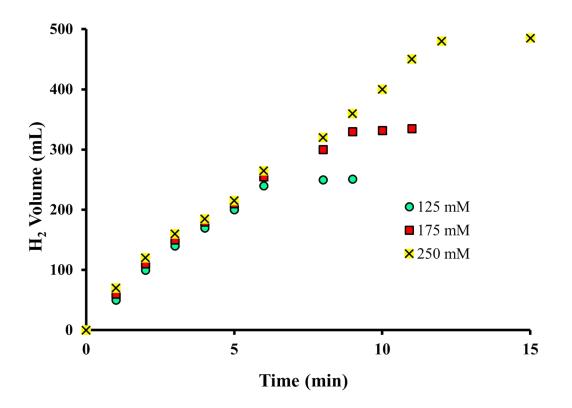


Figure S9. The effect of different concentrations of NaBH₄ on HGR over 2 mg of QT-300 at 25°C.

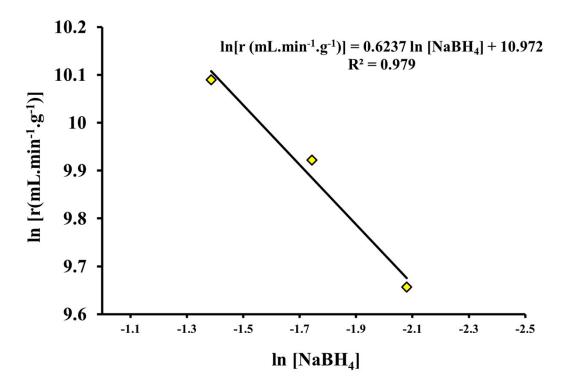


Figure S10. Plot of HGR versus the concentration of NaBH₄ (both in natural logarithmic scale) over QT-300 catalyst at 25 °C.

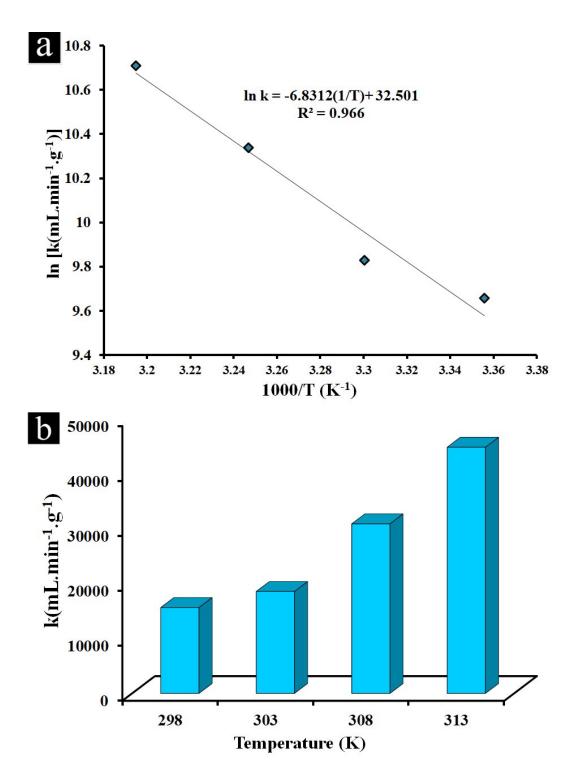


Figure S11. Temperature dependence of HGR over 2 mg of QT-300 catalyst, $[NaBH_4] = 125$ mM.

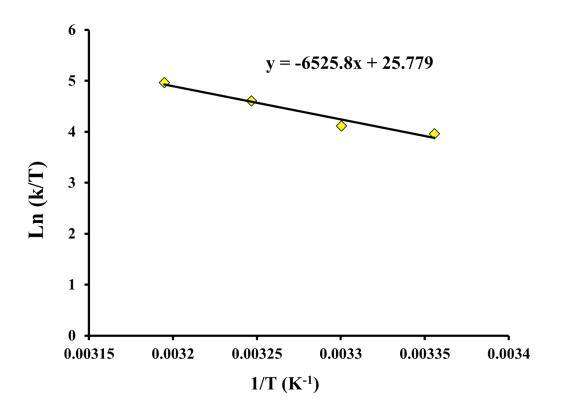


Figure S12 The Eyring plot for obtaining thermodynamic parameters on HGR over QT-300 catalyst.

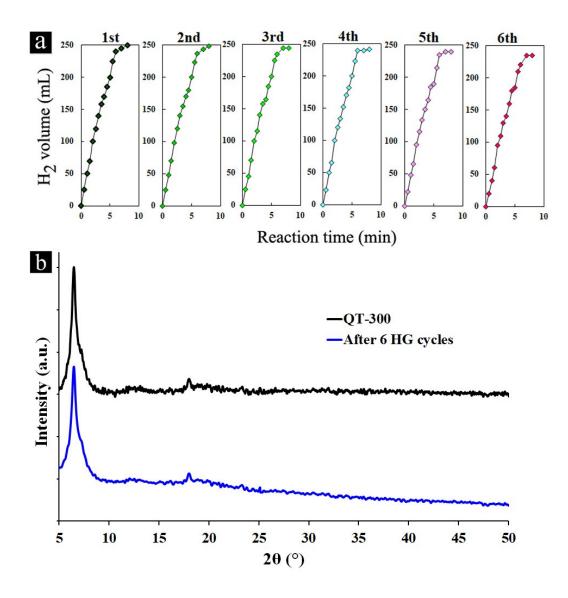


Figure S13 The reusability of the QT-300 catalyst on NaBH₄ hydrolysis at 25 °C for six catalytic cycles (a) and the XRD pattern of the QT-300 catalyst after six catalytic runs (b).

Table S1. BET surface area, total pore volume, micro- and mesopore volume of the synthesizedMOFs.

Sample	S_{BET} (m ² g ⁻¹)	V_t (cm ³ g ⁻¹)	V_{micro} (cm ³ g ⁻¹)	V_{meso} (cm ³ g ⁻¹)
TMU-10	8.2	0.023	0.004	0.023
QT-300	38.8	0.157	0.015	0.142

Table S2. Effect of QT-300 amount as a catalyst on TOF of NaBH₄ hydrolysis.

Entry	Catalyst dosage (mg)	TOF (ml min ⁻¹ g ⁻¹)	Time (min)
1	0	*1	60
2	1	8000	15
3	1.5	13333.3	10
4	2	15625	8
5	3	15555	6
6	3.5	15238	6
7	4	15250	5
7	5	15500	4

Experimental conditions: [NaBH₄] = 125 mM, T= 25 °C.*HGR in mLH₂.min⁻¹.