Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Elucidating, understanding and correlating the photo-electrochemical properties of HKUST-1 through a computational and experimental approach.

Table S1. Crystallite size determined for HKUST-1 synthesized in different works

Material	Crystallite size (nm)	Ref
$HKUST\text{-}1_{slow\ evaporation}$	123	This work
$HKUST\text{-}1_{5min}$	59	1
$HKUST\text{-}1_{10min}$	51	
$HKUST\text{-}1_{15min}$	57	
$HKUST\text{-}1_{20min}$	60	
Co-ferrite@HKUST-1	24	2
$HKUST\text{-}1_{MW}$	22.4	3
Ag_3PO_4/HKUST-1	20	
Ag/Ag_3PO_4/HKUST-1	24.40	
HKUST-1-0NH_2	36.7	4
HKUST-1-25NH_2	27.1	
HKUST-1-50NH_2	32.5	
HKUST-1-75NH_2	31.8	
HKUST-1-100NH_2	20.7	
HKUST-1-N1	58.3	5
HKUST-1-N2	51.9	
HKUST-1-N3	41.7	
HKUST-1-N4	49.3	
HKUST-1-N5	51.8	
HKUST-1-N6	70	
HKUST-1-T1	80.9	
HKUST-1-T1.5	60	
HKUST-1-T2	78.6	
HKUST-1-T3	68.5	
HKUST-1-C0	47.5	
HKUST-1-C1	42.4	
HKUST-1-C1.5	42.1	
HKUST-1-C3	57.4	
HKUST-1-C4	57	
$HKUST\text{-}1_{industrial\ production}$	87	6
$HKUST\text{-}1_{(C/route\ 20\ h)}$	~ 40	7
$HKUST\text{-}1_{(H/route\ 10\ h)}$	~ 85	
$HKUST\text{-}1_{(H/route\ 20\ h)}$	~ 83	
$HKUST\text{-}1_{(H/route\ 48\ h)}$	~ 44	
$HKUST\text{-}1_{(H1)}$	52.9	8
H1/G_A	45.1	

H1/G_B	49.5	
H1/G(Cu)_A	50.3	
H1/G(Cu)_B	43.3	
MOF-199(HKUST-1)	30.41	[9]
MOF-199/ $BaTi_{0.85}Zr_{0.15}O_3$(10%)	38.63	
MOF-199/ $BaTi_{0.85}Zr_{0.15}O_3$(20%)	41.76	
MOF-199/ $BaTi_{0.85}Zr_{0.1}O_3$(30%)	40.07	
HKUST-1	56.88	[10]
BF-PS	34.29	
$BF\text{-}OP_O$	40.25	
$BF\text{-}OP_M$	49.34	
CV-PS	40.47	
$CV\text{-}OP_O$	44.38	
$CV\text{-}OP_M$	44.41	
EBT-PS	37.35	
$EBT\text{-}OP_O$	40.57	
$EBT\text{-}OP_M$	44.41	

Table S2. Bandgap determined for HKUST-1 synthesized in different works

Material	Bandgap (eV)	Type of transition	Ref
$HKUST\text{-}1_{\text{slow evaporation}}$	3.30	Indirect	
$HKUST\text{-}1_{5min}$	3.55	Direct	[1]
$HKUST\text{-}1_{10min}$	3.42		
$HKUST\text{-}1_{15min}$	3.47		
$HKUST\text{-}1_{20min}$	3.45		
$HKUST\text{-}1_{solvothermal}$	3.5	Direct	[11]
$HKUST\text{-}1_{solvothermal\ (1)}$	3.31	Direct	[12]
$HKUST\text{-}1_{solvothermal\ (2)}$	2.81		[13]
$HKUST\text{-}1_{DMF/EtOH}$	3	-----	[14]
$HKUST\text{-}1_{DMF/EtOH\ (Ce/Eu)}$	2.60		
$HKUST\text{-}1_{ultrasoun\text{-}solvothermal}$	2.63	Direct	[15]
$HKUST\text{-}1_{MW}$	3.15	Direct	[3]
$HKUST\text{-}1_{computational}$	2	----	[16]
$HKUST\text{-}1_{solvothermal\ (3)}$	3.4	Direct	[17]
$HKUST\text{-}1_{solvothermal\ (H2O/EtOH)}$	3.32	Direct	[18]

Table S3. Mulliken charges and spin density calculated for HKUST-1. Here, minimum (min), averaged (aver), and maximum (max) charge values are reported.								
Compound	Elements	*s*	*p*	*d*	*f*	Total population	Charge (*e*)	Spin density
HKUST-1	Cu	6.403 6.403 6.403	12.339 12.337 12.337	9.305 9.305 9.302	0.00 0.00 0.00	28.047 28.045 28.042	+0.953 (min) +0.955(aver) +0.958 (max)	±0.5
	O	3.906 3.907 3.907	4.679 4.679 4.679	0.026 0.026 0.027	0.00 0.00 0.00	8.611 8.612 8.613	-0.611 (min) -0.612(aver) -0.613 (max)	±0.1
	C	3.181 3.157 2.975	2.873 2.790 2.199	0.035 0.032 0.116	0.00 0.00 0.00	6.089 5.979 5.290	-0.089 (min) 0.021 (aver) 0.710 (max)	0.0

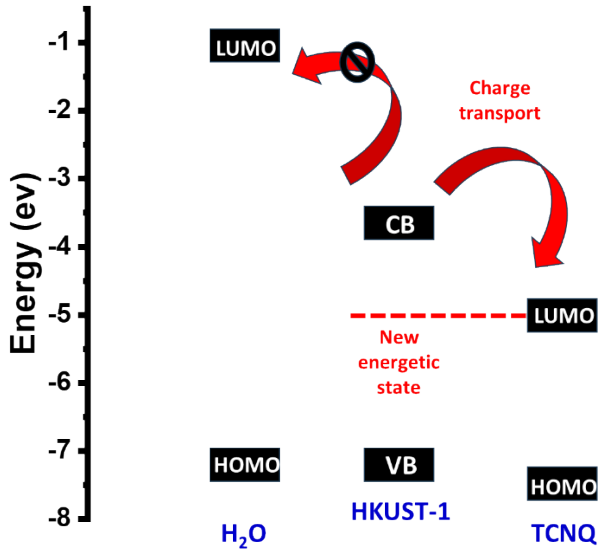

Figure S1. HOMO-LUMO energy of H_2O [19], VB and CB energy of HKUST-1, and HOMO-LUMO energy of TCNQ [20, 21].

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