Supporting Information

Heterobimetallic Ta-Nb MOF offering a moderated Lewis/Brønsted acidity expedites glucose isomerization to fructose under microwave conditions

Sangeeta Mahala,[1] Bhawana Devi,[1] Meera Cheviri,[1] Senthil Murugan Arumugam,[1] Balamurugan Arumugam,[2] Lakshmanan Potturaja,[1] Vishnu Bakthavachalam,[1] Joy K. Roy,[3] and Sasikumar Elumalai[1,*]

[1] *Chemical Engineering Division, DBT-Center of Innovative and Applied Bioprocessing, Mohali, Punjab 140306 India*

[2] *Department of Chemistry, Sri Manakula Vinayagar Engineering College, Madagadipet, Puducherry 605107 India*

[3] *Agricultural Biotechnology Division, DBT-National Agri-Food Biotechnology Institute, Mohali, Punjab 140306 India*

[*]Corresponding author information: sasikumar@ciab.res.in (S. Elumalai)
Tel: +91-172-5221-444

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Experimental

Mathematical expressions

$$Glucose/Fructose\ conversion\ (\%) = \frac{(Intial\ wt.\ of\ sugar - Remaining\ wt.\ of\ sugar\ after\ completio}{Intial\ wt.\ of\ sugar} \times 100$$

---------- (S1)

$$Product\ yield\ (\%) = \frac{Product\ weight}{Initial\ glucose\ weight} \times 100$$

---------- (S2)

$$Product\ selectivity\ (\%) = \frac{Product\ weight}{Converted\ glucose\ in\ weight} \times 100$$

---------- (S3)

First-order kinetic rate equation

$$ln\left\{\frac{[Sugar]_t}{[Sugar]_0}\right\} = -\ k \times time\ (sec)$$

---------- (S4)

Where, sugar can be glucose or fructose. $[Sugar]_t$ and $[Sugar]_0$ represent the final and initial reactant (sugar) concentration at time *t*. *k* is the observed rate constant of reaction (disappearance of sugar).

The temperature dependency of the rate constant, *k* was determined by using the Arrhenius equation (Eqn. S5):

$$k = A_0 \times e^{\left(-\frac{E_a}{RT}\right)}$$

---------- (S5)

where, A_0 is the frequency factor (or Arrhenius constant), E_a is the activation energy (J/mol), and *R* is the universal gas constant (8.31 J/mol. K).

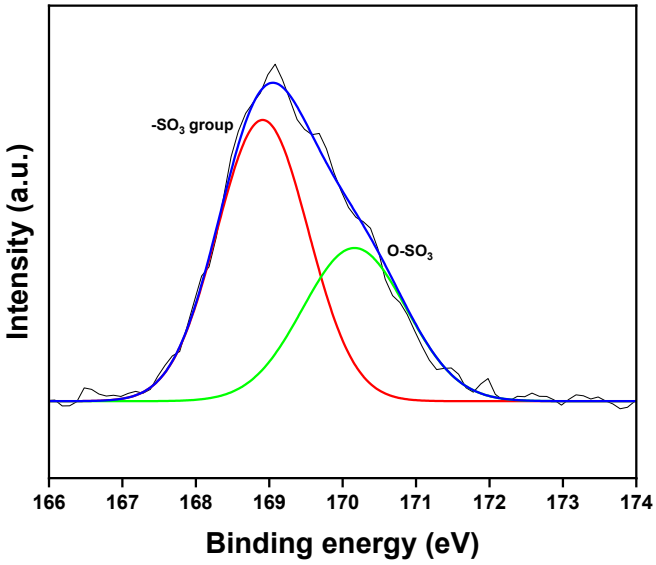

Figure S1. Deconvolution result of S 2p spectra of S-Ta MOF catalyst.

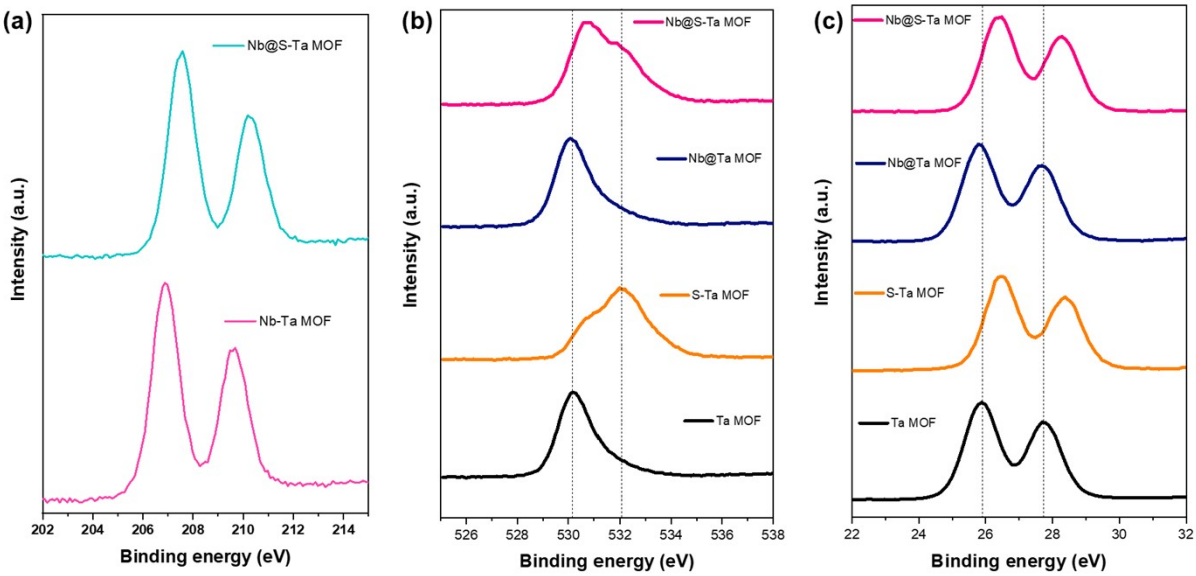

Figure S2. Comparative XPS result (a) Nb 3d spectra of Nb-Ta MOF and Nb@S-Ta MOF(b) O1s spectra of Ta MOF, S-Ta MOF, Nb@Ta MOF and Nb@S-Ta MOF (c)Ta 4f spectra of Ta MOF, S-Ta MOF, Nb@Ta MOF and Nb@S-Ta MOF catalyst.

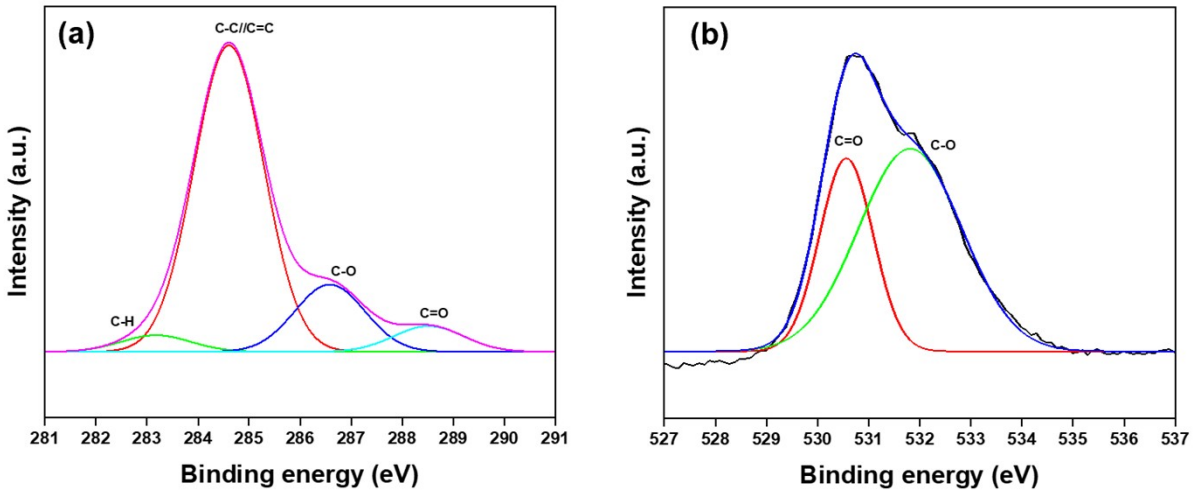

Figure S3. XPS deconvolution result of (a) C 1s and (b) O 1s spectra of Nb@S-Ta MOF catalyst.

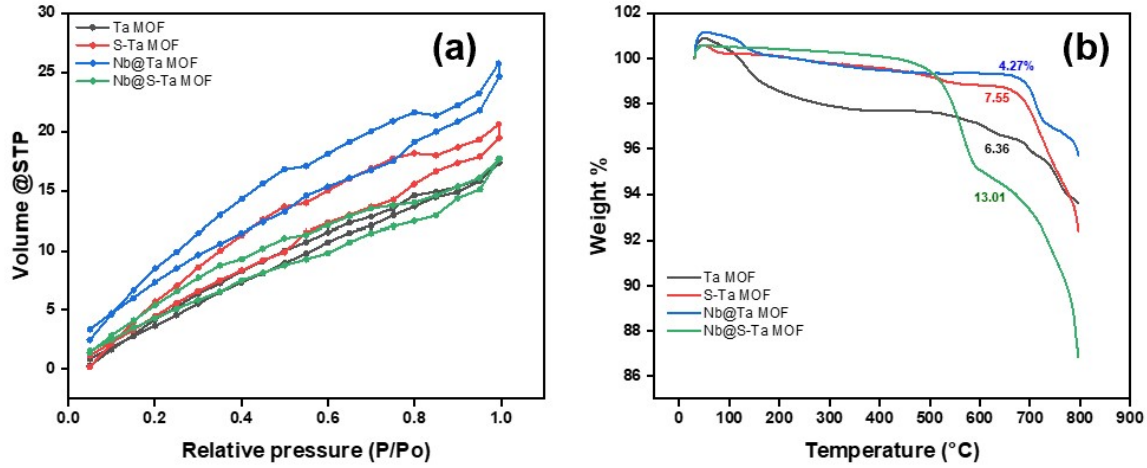

Figure S4. (a) N_2 adsorption/desorption isotherm and (b) TGA report of MOF catalysts.

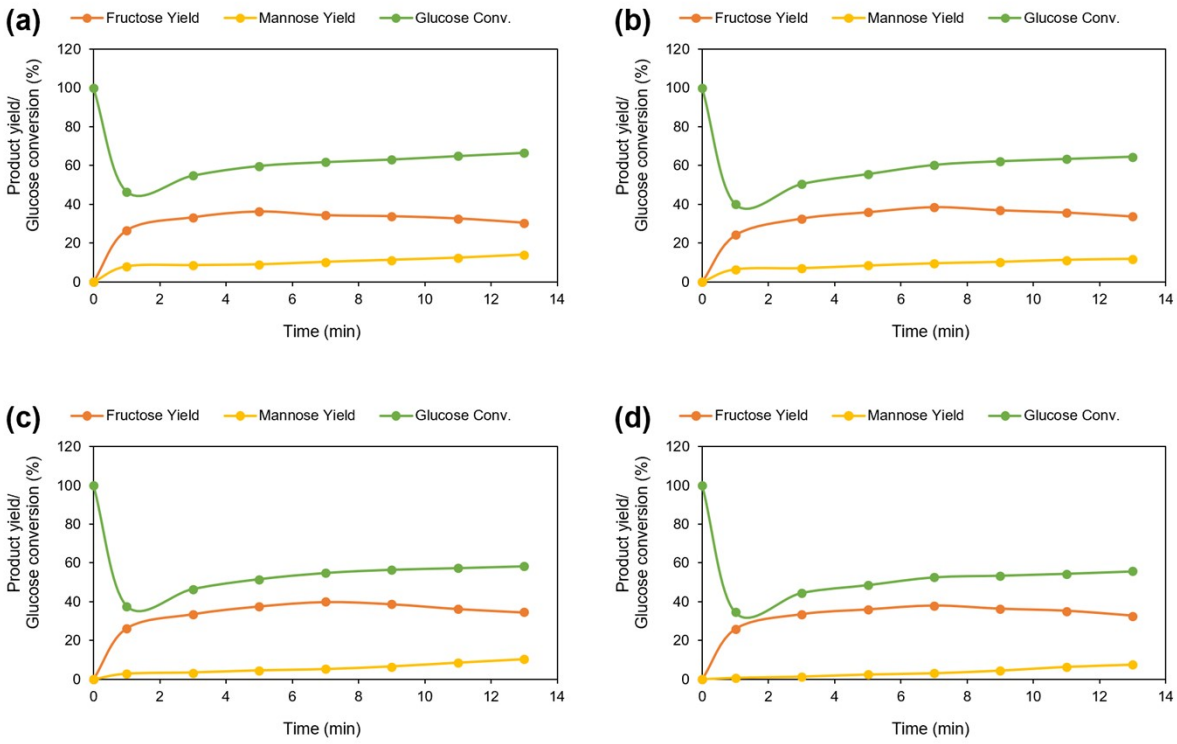

Figure S5. Glucose consumption and product(s) formation profile (fructose and mannose) with respect to change in Nb@S-Ta MOF loading on glucose under microwave conditions in a water medium: (a) 25%, (b) 50%, (c) 75% and (d) 100% at 100 °C up to 13 min.

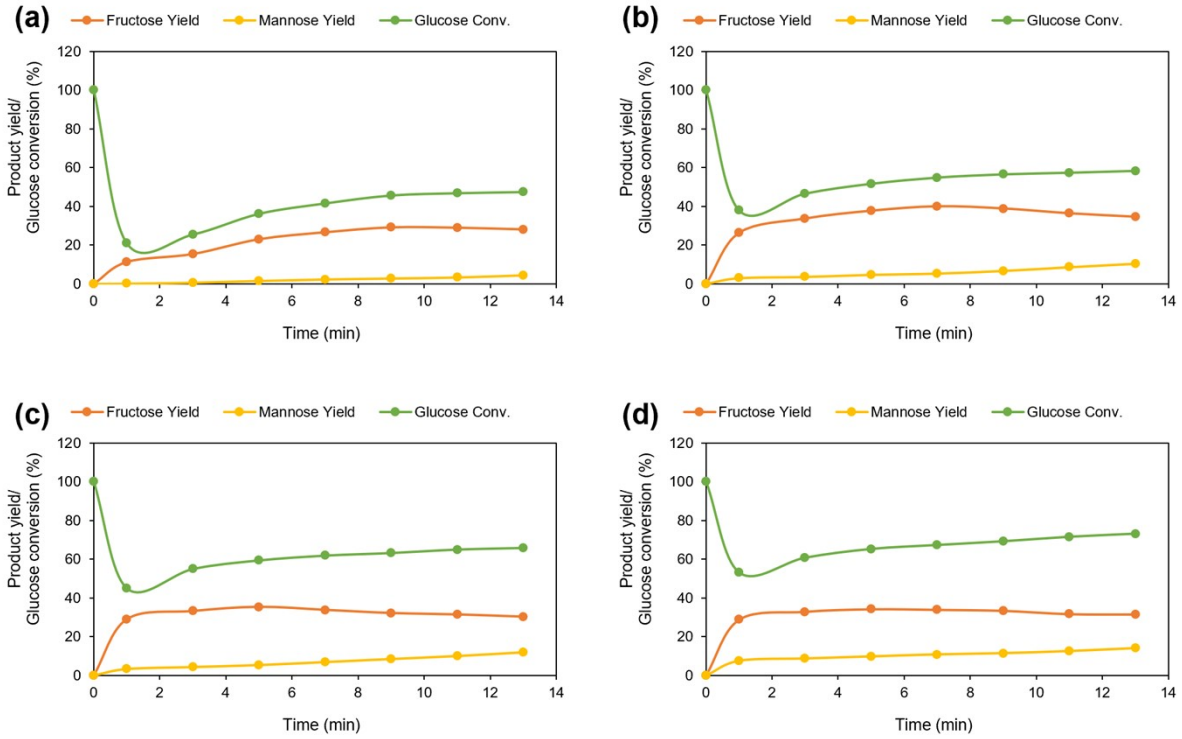

Figure S6. Glucose consumption and product(s) formation profile (fructose and mannose) with respect to change in temperature over Nb@S-Ta MOF under microwave conditions in a water medium: (a) 90 °C, (b) 100 °C, (c) 110 °C and (d) 120 °C at 50% catalyst load on glucose up to 13 min.

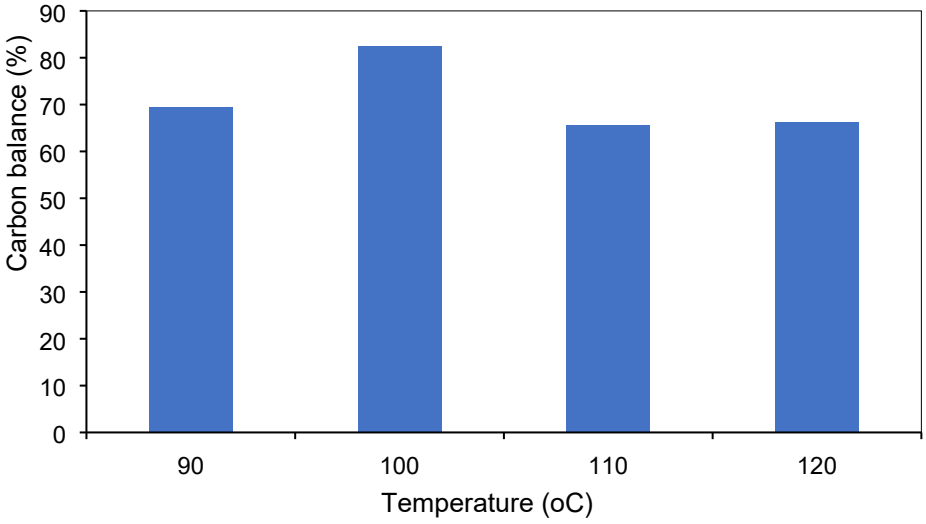

Figure S7. Carbon balance (CB) data of the effect of temperature (90-120 °C) on glucose isomerization to fructose over Nb@S-Ta MOF under microwave conditions in a water medium. Note: CB was made by relating the moles of carbon produced to the moles of carbon in the reactant.

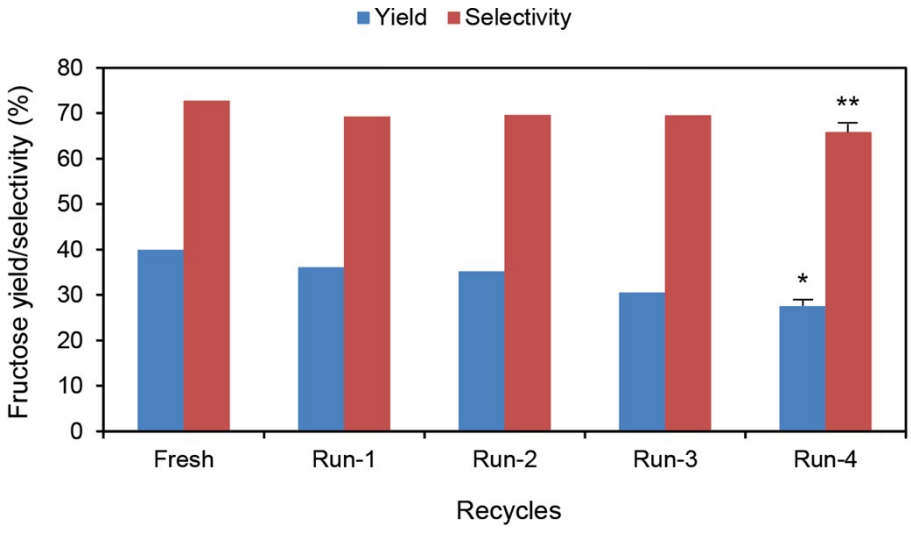

Figure S8. Result of recyclability of Nb@S-Ta MOF for glucose conversion to fructose under microwave conditions in a water medium at 100 °C at 50% catalyst load on glucose.

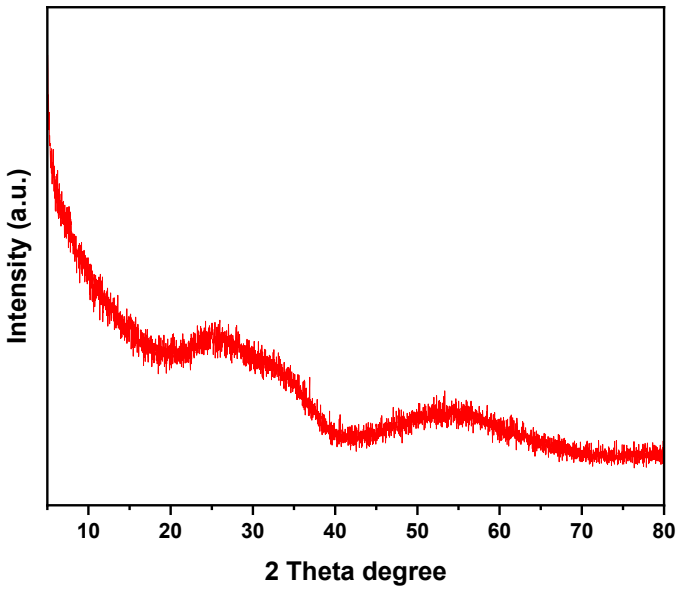

Figure S9. XRD result recycled Nb@S-Ta MOF after 5 runs (including a fresh run) of glucose conversion to fructose under microwave conditions in a water medium at 100 °C at 50% catalyst load on glucose.

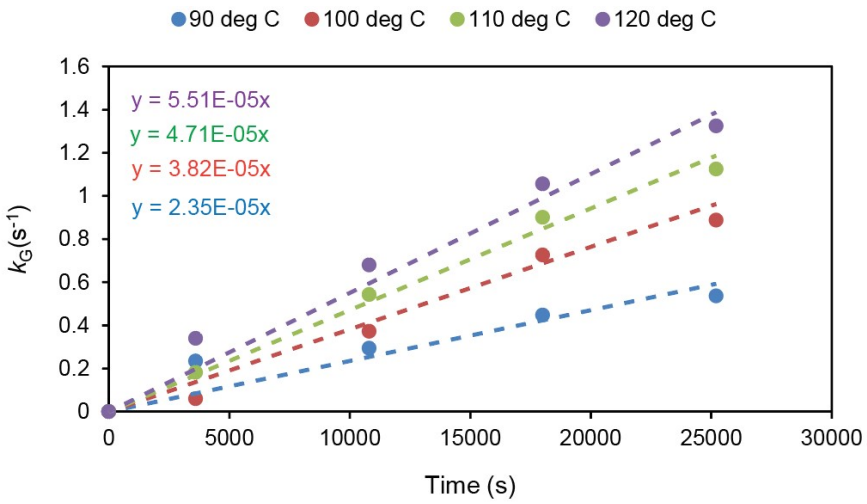

Figure S10. First-order model fitting of rate constant (k_G) at different temperatures (90-120 °C).

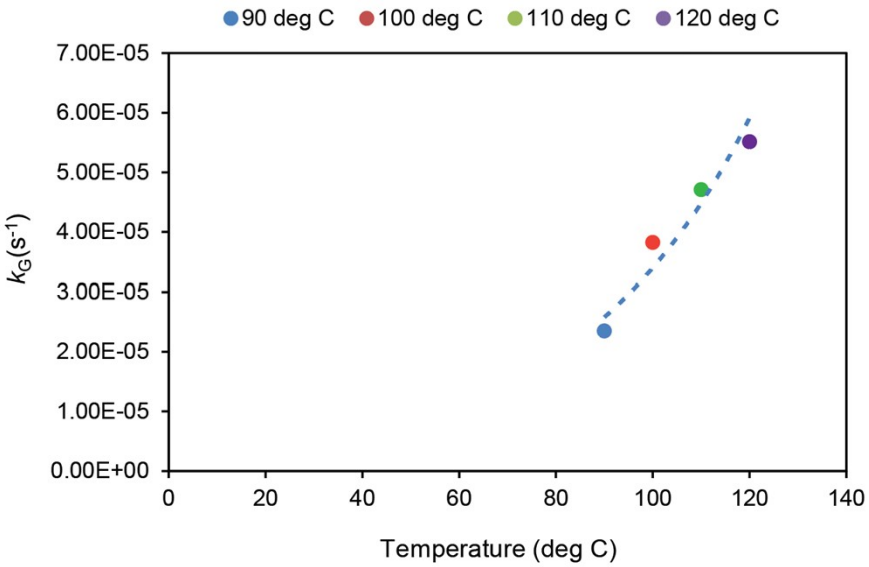

Figure S11. Correlation plot of rate constant (k_G) *vs*. temperature (90-120 °C).

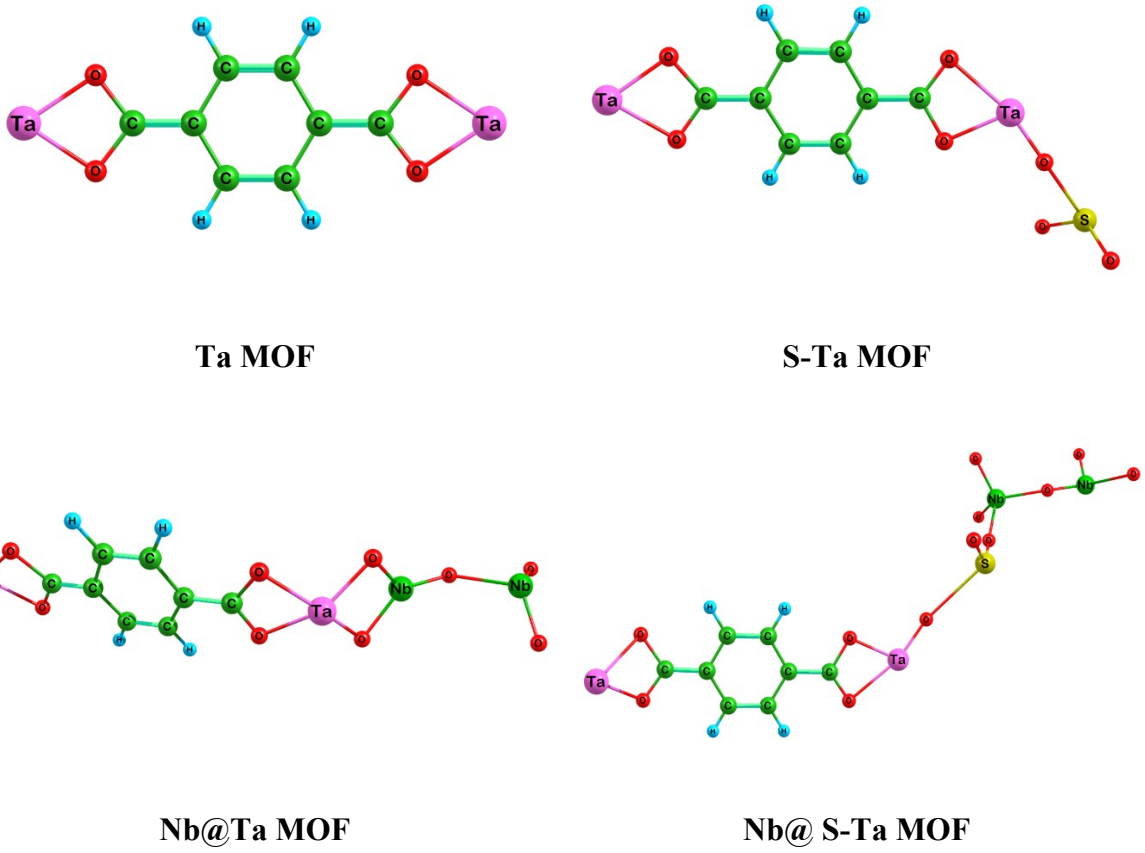

Figure S12. DFT optimized structures of various MOFs for calculating the binding energy using VASP software.

Table S1. Determined *x, y* and *z* coordinates of MOF catalysts during DFT modeling.

	x	*y*	*z*
Ta MOF			
Ta	7.049214009000	7.424328469000	15.287049043043
Ta	7.049214009000	7.424328469000	4.781758900957
O	6.284396785138	8.189145692862	13.663842301073
O	7.814031232862	6.659511245138	6.404965642927
O	6.284396785138	8.189145692862	6.404965642927
O	7.814031232862	6.659511245138	13.663842301073
C	7.049214009000	7.424328469000	12.832149489974
C	7.049214009000	7.424328469000	11.454475874169
C	6.173851678727	8.299690799273	10.716093901959
C	7.049214009000	7.424328469000	7.236658454026
C	7.049214009000	7.424328469000	8.614332069831
C	7.924576339273	6.548966138727	9.352714042041
C	6.173851678727	8.299690799273	9.352714042041
C	7.924576339273	6.548966138727	10.716093901959
H	5.509650195766	8.963892282234	11.269110932965
H	8.588777822234	5.884764655766	8.799697011035
H	5.509650195766	8.963892282234	8.799697011035
H	8.588777822234	5.884764655766	11.269110932965
S-Ta MOF			
Ta	6.628819171467	6.848656808548	15.272277386709
Ta	7.094900570271	7.438126860604	4.932316680963
S	7.177054808687	7.276376778141	19.596095329386
O	6.276941196646	8.176109582526	13.800506289545
O	7.840596986235	6.674531186639	6.558797658315
O	6.313983174104	8.208725949900	6.539720057537
O	7.874992081301	6.621370616654	13.738661661555
O	6.314082693174	6.134529833308	19.839545040780
O	8.590745206166	7.137537481679	19.884507910967
O	7.259700168754	7.282175155644	16.843660789562
C	7.069124168596	7.427885898804	12.988862563827
C	7.044808692362	7.424571248233	11.595067741722
C	6.179083089491	8.304791983305	10.863967831634
C	7.064241202591	7.440030422013	7.379987589513
C	7.051485816608	7.435879781538	8.760989124824
C	7.924808490653	6.559494541955	9.494663015485
C	6.177868317100	8.309940878818	9.497371159875
C	7.922778108752	6.559053455135	10.859787094431
H	5.518236119616	8.969801693190	11.419405658464
H	8.588141210101	5.893476127857	8.943840359959
H	5.514662173335	8.977779638742	8.948227992206
H	8.585575163990	5.893829779768	11.412631145741

Nb@Ta MOF

Ta	7.209568228330	7.234308522021	15.208143627325
Ta	7.092804021219	7.483695896680	4.702133737297
Nb	8.613728628828	8.118366142426	17.516192427999
Nb	9.204631596072	8.501357296437	21.084415123721
O	6.341765075853	8.076399419381	13.552183376000
O	7.836231555182	6.684366899222	6.301799421655
O	6.347388530182	8.246548059822	6.320243621768
O	7.785166037764	6.397548452018	13.460899502413
O	7.174685353689	8.734262508791	16.446139067797
O	8.516195187527	6.531018070322	16.461858260103
O	9.393884556290	8.725778500236	19.120163390883
O	10.459168755893	9.247974624518	22.026862107639
O	9.079549269892	6.831267142686	21.553063977154
C	7.033138547566	7.260089863777	12.744949145498
C	7.030862160328	7.312424918075	11.352057492585
C	6.200509478421	8.242671707433	10.646699915516
C	7.081356218807	7.446601924233	7.148140049528
C	7.059224608183	7.406168317768	8.526871005008
C	7.896725617255	6.478209923086	9.238431376835
C	6.208648487628	8.288941525786	9.280978336510
C	7.876766996760	6.432735665621	10.602365460496
H	5.565602117129	8.916207441452	11.221932804825
H	8.548855176728	5.816258967823	8.669618235897
H	5.579246466771	8.999586542871	8.746148578459
H	8.511544521705	5.731409565514	11.142776663091

Nb@S-Ta MOF

Ta	7.260490796554	10.800402687196	13.932471106522
Ta	7.752426280232	12.065814002349	4.113824546406
Nb	9.500589036644	4.939463950851	17.935257022370
Nb	10.042014091117	4.390089308330	21.636218217847
S	9.797865783931	8.352487773964	16.730028062196
O	6.332650486167	11.983252194198	12.217701356652
O	7.572443260748	10.344832138576	4.970299665952
O	6.038836838687	12.016153245292	5.004065017795
O	7.822580898662	10.326605007345	12.119647726523
O	9.422185512948	7.001581000165	17.260636984534
O	10.980052563441	8.384792558770	15.897412817585
O	8.042749278008	9.595710532023	14.911133205051
O	7.847145513636	4.368759214064	17.890958973889
O	10.458958409442	3.893419623448	16.919167151673
O	10.112870875234	4.934217042547	19.806143264883
O	11.325141555109	5.103468904706	22.574453907355
O	10.114033431650	2.665064228356	21.859564201755
C	7.039756468925	11.237646251889	11.463041615947
C	7.053214715855	11.269349852960	10.024369851559
C	6.192625221521	12.163227157540	9.341810048329
C	6.900744924587	11.251948118399	5.801081229765
C	6.989607715169	11.300715870025	7.223595496715

C	7.865225912349	10.421018627037	7.905971147695
C	6.156722244628	12.179128498048	7.961348495538
C	7.894582900765	10.405097069027	9.286590447226
H	5.553056980075	12.826970362488	9.923204498052
H	8.499278179922	9.748163356263	7.329269874373
H	5.483846653415	12.850126127503	7.428506048923
H	8.558137059579	9.723253303640	9.817142920888