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Supporting Information

Computer modelling of SO_2 and NO_2 capture and conversion in flue gases by optimised Zn(II) MOF catalysts.

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1. DFT optimized structures of HbMOF series with various ligands:

In the partially fluorinated HbMOF-1, it contains long-chain dicarboxylate ligand and melamine as a co-ligand utilizing Zinc as a metal centre. From here, we designed three more hypothetical frameworks by exchanging the ligands.

1.1. Density Functional Theory Calculations:

The obtained series of HbMOF were optimized through PBE[1-2] functional via the DFT theory implemented in CP2K package[3]. The DFT calculations were performed by Unrestricted Kohn-Sham with spin multiplicity[4]. For carbon, nitrogen, oxygen, and fluorine atoms in the framework, triple zeta (TZVP-MOLOPT) were considered and for Zinc atom double zeta (DZVP-MOLOPT) was considered as the basis set[5]. Further van der walls corrections were applied via the DFT-D3 method[6].

1.2. Inter atomic potential:

The overall interaction that occurred between the MOFs and guest molecules were modelled via a combination of Lennard-Jones and columbic term. For the simulation adsorption isotherm, we have implemented DRIEDING[7] and UFF[8] force fields. We have used the UFF force field for the transition metals and DRIEDING for all other atoms in the framework. In this work, all the LJ parameters were elucidated by UFF and DRIEDING forcefield potentials for all the simulations. Here, the NO_2 modelled from the work of Bourasseau *et al*[9] model and SO_2 from the used model of Potoff *et al*[10]. The atomic point charges for all the frameworks were obtained from the REPEAT method suggested by Campana et al[11]. which is successfully implemented in the CP2K package.

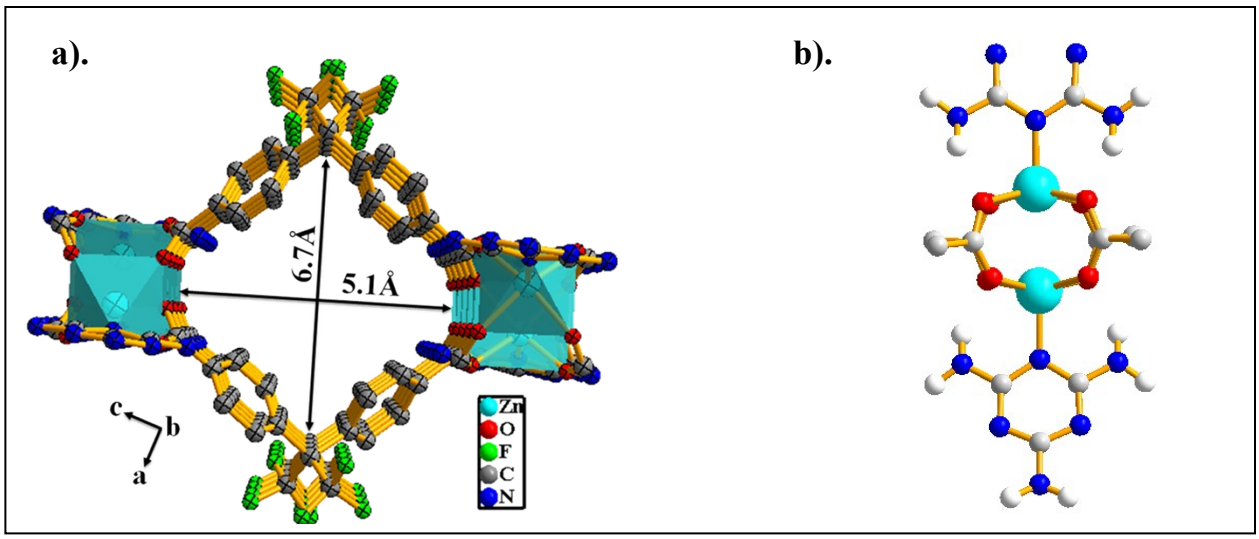


Figure S1: Graphical representation of (a) Pore channel of HbMOF1, and (b) a 4-connected view of paddle wheel Zn(II) metal site with the carboxylate linker.

Table S1. LJ potential parameters for all the atoms of HbMOF series:

Atom type	**LJ**	
	ε / k_B **(K)**	**σ (Å)**
C	47.857	3.4730
H	7.6490	2.8460
N	34.724	3.6620
O	30.190	3.1200
F	38.975	3.0930

Zn	27.680	4.0500

Table S2. Partial charges for all the atoms of HbMOF1 derived by REPEAT method:

Interaction atoms/sites	**Charge** *q (e)*
C1	0.615
C2	-0.453
C3	0.373
C3A	-0.134
C4	0.003
C4A	-0.0642
C5	0.5990
C6	0.883
H1	0.395
H2	0.268
H3	0.252
N1	-0.556
N2	-0.718

N3	-0.697
N4	-1.073
Zn1	0.909
O1	-0.434
F1	-0.168

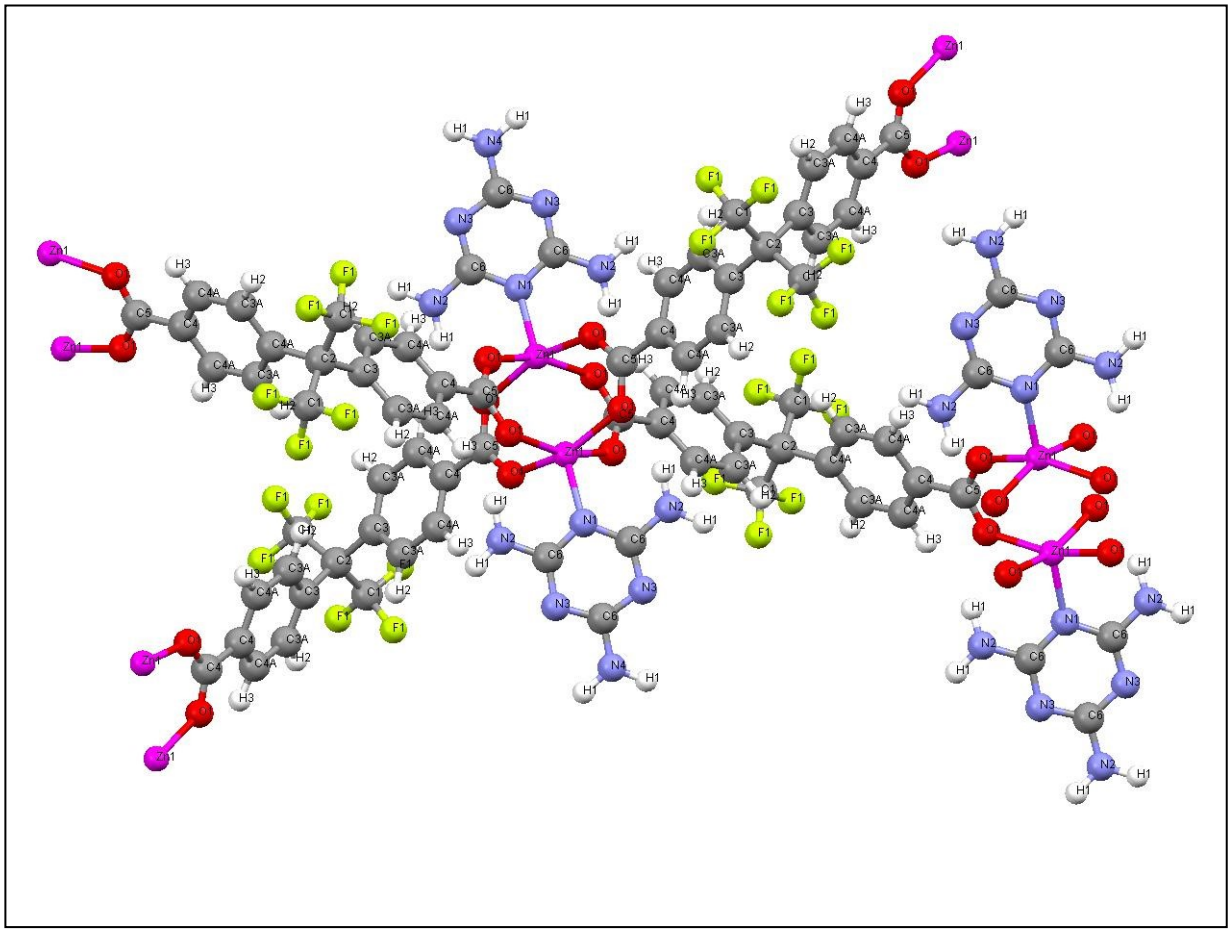


Figure-S2: Labels of the atoms for the HbMOF1 framework.

1.3. GCMC simulations:

The simulated adsorption isotherm for the toxic gases such as NO_2 and SO_2 on the HbMOF series were carried out via the Grand canonical Monte Carlo method and the simulations were conducted at the 298K and the pressure ranging from 0.1 to 1 bar using RASPA code[12]. The model corresponds to adsorbate and the dispersion forces in short ranges were explained with the help of Lennard–Jones potential parameters and the Ewald method was applied for coulombic interaction. within the cutoff of 12 Å. The fugacity of species was calculated via the Peng-Robinson equation of states[13]. The adsorption enthalpy (ΔH) was calculated based on the NVT ensemble by using revised Wisdom's test particle insertion method[14].

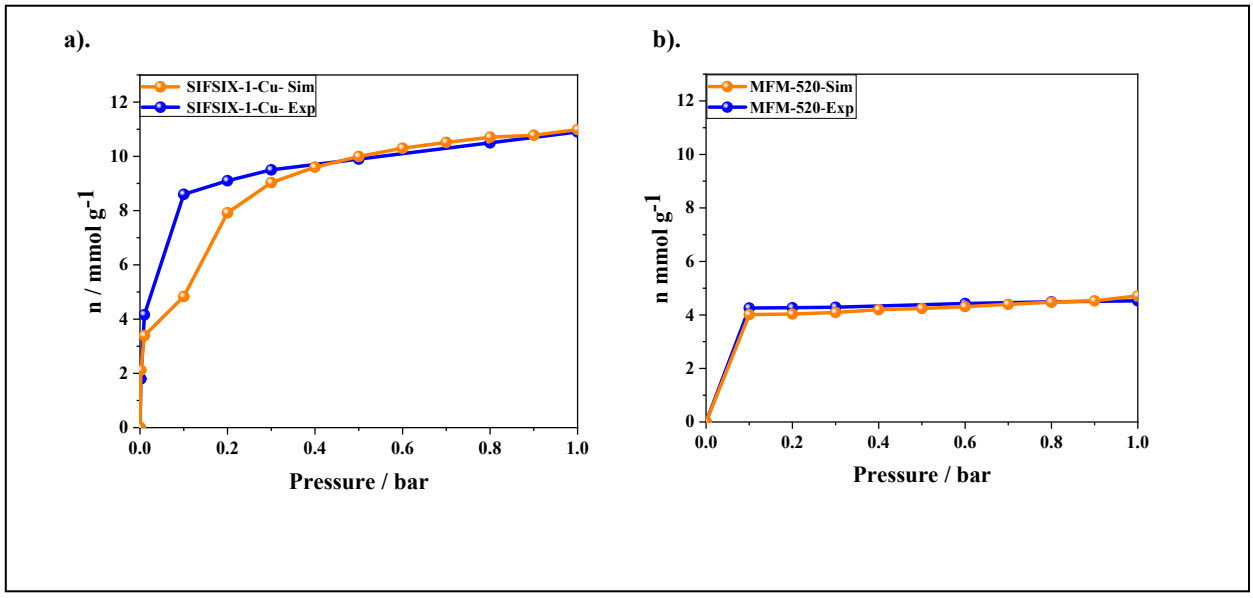


Figure S3: Comparison between the simulated and experimental adsorption isotherm of SO_2 (a) gas on SIFSIX-1-Cu and NO_2 (b) gas on MFM-520 using three site gas model.

1.4. Atomic Co-ordinates HbMOF series:

Table S3: Atomic coordinates of HbMOF1

Zn1	0.54668	0.11653	0.98511
O1	0.67722	0.03608	0.02031
O1	0.6073	0.86157	0.03636
F1	0.12769	0.93082	0.17041
O1	0.99971	0.64875	0.42308
F1	0.03366	0.55326	0.08318
C1	0.09862	0.64658	0.08245
C1	0.15596	0.83367	0.13835
O1	0.05611	0.46557	0.39935
F1	0.23842	0.78656	0.16969
C4	0.78099	0.88625	0.06106
N1	0.59549	0.28461	0.96671
F1	0.19376	0.60361	0.09327
N3	0.5699	0.46294	0.90729
C3A	0.10339	0.58266	0.21709
H2	0.14728	0.52959	0.18627
C3A	0.88024	0.73106	0.11193
H2	0.88395	0.64506	0.1349
F1	0.09427	0.69141	0.02361
N3	0.65495	0.47049	0.00875
F1	0.18465	0.874	0.08272
N2	0.51488	0.2826	0.8685
H1	0.49672	0.32738	0.82883
H1	0.52405	0.1927	0.86667
C4A	0.96874	0.79706	0.10604
N2	0.69028	0.29567	0.06047
H1	0.73623	0.34537	0.08891
H1	0.70014	0.20616	0.05926
C4	0.04157	0.61178	0.31985
C3A	0.96196	0.90795	0.07666
H2	0.02886	0.96176	0.07058
C4A	0.8689	0.95233	0.05498
H3	0.86395	0.03288	0.03266
C4A	0.09429	0.54418	0.27801
H3	0.12962	0.46159	0.29361
C3A	0.0049	0.75631	0.23885
H2	0.96953	0.83958	0.22393
C4A	0.99655	0.71862	0.29974

H3	0.95521	0.77122	0.3323
C2	0.0691	0.74135	0.13126
C5	0.68097	0.93388	0.03749
C4A	0.78763	0.77447	0.08946
H3	0.71955	0.72231	0.0943
C5	0.03181	0.57239	0.38559
C3	0.05802	0.68887	0.19664
N2	0.6156	0.64108	0.9533
H1	0.63311	0.68906	0.99238
H1	0.57093	0.68243	0.92033
C6	0.64676	0.3525	0.01075
C6	0.61247	0.52155	0.95683
C6	0.56171	0.34585	0.91492
Zn1	0.95665	0.62494	0.51434
O1	0.82727	0.54657	0.47023
O1	0.89348	0.36306	0.46012
F1	0.37205	0.42782	0.32928
O1	0.50673	0.13746	0.07713
F1	0.46629	0.05025	0.41668
C1	0.40145	0.14365	0.41742
C1	0.34397	0.3305	0.36135
O1	0.44418	0.96289	0.10046
F1	0.26139	0.28352	0.33018
C4	0.72162	0.38953	0.43076
N1	0.90512	0.79091	0.53369
F1	0.30629	0.10066	0.40656
N3	0.93281	0.96897	0.59302
C3A	0.39683	0.07653	0.28265
H2	0.35406	0.02268	0.31372
C3A	0.62118	0.23076	0.38393
H2	0.61741	0.14332	0.36262
F1	0.40566	0.18849	0.47614
N3	0.84701	0.97728	0.49205
F1	0.31571	0.37089	0.41699
N2	0.97832	0.78728	0.63415
H1	0.99388	0.83217	0.67418
H1	0.96992	0.69716	0.6349
C3	0.53176	0.29523	0.39129
N2	0.81065	0.80332	0.43983
H1	0.76359	0.85343	0.41233
H1	0.80039	0.71367	0.4411
C4	0.4596	0.10392	0.17972
C3A	0.53912	0.40743	0.41871
H2	0.47279	0.46021	0.42641
C4A	0.63293	0.4548	0.43769

H3	0.63828	0.54306	0.45787
C4A	0.40685	0.03675	0.22197
H3	0.37217	0.95946	0.20683
C3A	0.49172	0.25195	0.25963
H2	0.52507	0.3364	0.27364
C4A	0.50141	0.21262	0.19916
H3	0.54246	0.2659	0.16676
C2	0.43091	0.2379	0.36801
C5	0.82181	0.43717	0.45524
C4A	0.71446	0.27676	0.40351
H3	0.78278	0.22521	0.3984
C5	0.47127	0.0629	0.1143
C3	0.44045	0.18424	0.30252
N4	0.89327	0.14092	0.54548
H1	0.86872	0.18987	0.50822
H1	0.9316	0.18362	0.58063
C6	0.85457	0.8595	0.48978
C6	0.89167	0.02202	0.54327
C6	0.93735	0.8515	0.58615
Zn1	0.45239	0.88385	0.01492
O1	0.32239	0.96853	0.97968
O1	0.3928	0.14268	0.96323
F1	0.87204	0.07467	0.82987
O1	0.01008	0.36403	0.57691
F1	0.96591	0.45271	0.91657
C1	0.90117	0.35927	0.91736
C1	0.84437	0.1702	0.8634
O1	0.94352	0.54245	0.59973
F1	0.76047	0.21397	0.83313
C4	0.21896	0.11872	0.93893
N1	0.40404	0.71551	0.03326
F1	0.80584	0.40238	0.90646
N3	0.42812	0.53654	0.09239
C3A	0.8987	0.42431	0.7827
H2	0.85729	0.47971	0.81399
C3A	0.11993	0.27401	0.88772
H2	0.11657	0.36004	0.86479
F1	0.90529	0.31468	0.97619
N3	0.34396	0.53022	0.99077
F1	0.8162	0.13164	0.91966
N2	0.47818	0.71622	0.13364
H1	0.49268	0.67013	0.17342
H1	0.47086	0.80642	0.13501
C4A	0.03131	0.20845	0.89374
N2	0.30922	0.70538	0.93925

H1	0.26103	0.65615	0.91201
H1	0.29785	0.79466	0.94158
C4	0.95977	0.39552	0.67941
C3A	0.03803	0.09763	0.92336
H2	0.97113	0.04399	0.92972
C4A	0.13089	0.05302	0.94513
H3	0.13564	0.97251	0.96756
C4A	0.90835	0.46358	0.72186
H3	0.87427	0.54755	0.70679
C3A	0.99184	0.24781	0.75979
H2	0.02554	0.16316	0.77406
C4A	0.00165	0.28679	0.69919
H3	0.04233	0.23309	0.66668
C2	0.93054	0.26395	0.86869
C5	0.31909	0.07087	0.96239
C4A	0.21245	0.23031	0.91035
H3	0.28054	0.28231	0.90546
C5	0.97163	0.43682	0.61379
C3	0.94074	0.31589	0.80271
N2	0.38399	0.35907	0.04564
H1	0.36655	0.31099	0.00667
H1	0.42741	0.31778	0.07918
C6	0.35271	0.64797	0.98906
C6	0.38649	0.47846	0.04259
C6	0.43538	0.65381	0.08566
Zn1	0.04715	0.38623	0.4849
O1	0.17793	0.46573	0.52016
O1	0.11079	0.64717	0.53674
F1	0.62765	0.59008	0.67646
O1	0.4893	0.865	0.9226
F1	0.53336	0.95645	0.58299
C1	0.59847	0.8636	0.58222
C1	0.65731	0.68056	0.6399
O1	0.5556	0.0377	0.89953
F1	0.73925	0.72967	0.67003
C4	0.28379	0.62027	0.56092
N1	0.09809	0.21937	0.46598
F1	0.69361	0.90582	0.5931
N3	0.07213	0.04011	0.40736
C3A	0.60664	0.92446	0.71874
H2	0.65361	0.97587	0.68886
C3A	0.38172	0.7776	0.61064
H2	0.38459	0.86452	0.63265
F1	0.59407	0.81772	0.52355
N3	0.15748	0.03412	0.50843

F1	0.68864	0.63501	0.58634
N2	0.02248	0.21997	0.36601
H1	0.00842	0.1743	0.32608
H1	0.02925	0.31013	0.36468
C3	0.47048	0.71183	0.60575
N2	0.194	0.2095	0.55922
H1	0.24035	0.16026	0.58765
H1	0.2035	0.29909	0.55756
C4	0.53923	0.89746	0.82039
C3A	0.46486	0.59975	0.57753
H2	0.53165	0.54577	0.57232
C4A	0.37201	0.55429	0.55582
H3	0.36791	0.46686	0.5343
C4A	0.59763	0.96161	0.77992
H3	0.63748	0.03432	0.79702
C3A	0.49968	0.75699	0.7379
H2	0.46184	0.67602	0.72207
C4A	0.4911	0.79363	0.79893
H3	0.44682	0.74231	0.83059
C2	0.56924	0.76992	0.63118
C5	0.18347	0.57358	0.5375
C4A	0.2896	0.73291	0.58838
H3	0.22123	0.78472	0.59265
C4	0.52726	0.93841	0.88572
C3	0.55665	0.82224	0.69669
N4	0.11666	0.86883	0.45437
H1	0.13562	0.82146	0.49335
H1	0.0731	0.82626	0.42131
C6	0.14947	0.15194	0.50998
C6	0.11422	0.98832	0.45714
C6	0.06561	0.1576	0.4139

Table S4: Atomic co-ordinates for HbMOF2:

Zn1	0.54668	0.11653	0.98511
O4	0.67722	0.03608	0.02031
O1	0.6073	0.86157	0.03636
F1	0.12769	0.93082	0.17041
O1	0.99971	0.64875	0.42308
F1	0.03366	0.55326	0.08318
C5	0.09862	0.64658	0.08245
C5	0.15596	0.83367	0.13835

O1	0.05611	0.46557	0.39935
F1	0.23842	0.78656	0.16969
C3	0.78099	0.88625	0.06106
N1	0.59549	0.28461	0.96671
F1	0.19376	0.60361	0.09327
N1	0.5699	0.46294	0.90729
C3	0.10339	0.58266	0.21709
H2	0.14728	0.52959	0.18627
C3	0.88024	0.73106	0.11193
H2	0.88395	0.64506	0.1349
F1	0.09427	0.69141	0.02361
N2	0.65495	0.47049	0.00875
F1	0.18465	0.874	0.08272
H1	0.53712	0.29582	0.87643
C3	0.96874	0.79706	0.10604
H4	0.67434	0.32358	0.04598
C3	0.04157	0.61178	0.31985
C3	0.96196	0.90795	0.07666
H6	0.02886	0.96176	0.07058
C3	0.8689	0.95233	0.05498
H6	0.86395	0.03288	0.03266
C3	0.09429	0.54418	0.27801
H2	0.12962	0.46159	0.29361
C3	0.0049	0.75631	0.23885
H6	0.96953	0.83958	0.22393
C9	0.99655	0.71862	0.29974
H5	0.95521	0.77122	0.3323
C4	0.0691	0.74135	0.13126
C2	0.68097	0.93388	0.03749
C3	0.78763	0.77447	0.08946
H2	0.71955	0.72231	0.0943
C2	0.03181	0.57239	0.38559
C3	0.05802	0.68887	0.19664
H1	0.62002	0.61194	0.95906
C8	0.64676	0.3525	0.01075
C1	0.61247	0.52155	0.95683
C1	0.56171	0.34585	0.91492
Zn1	0.95665	0.62494	0.51434
O1	0.82727	0.54657	0.47023
O2	0.89348	0.36306	0.46012
F1	0.37205	0.42782	0.32928
O3	0.50673	0.13746	0.07713
F1	0.46629	0.05025	0.41668
C5	0.40145	0.14365	0.41742
C5	0.34397	0.3305	0.36135

O1	0.44418	0.96289	0.10046
F1	0.26139	0.28352	0.33018
C3	0.72162	0.38953	0.43076
N1	0.90512	0.79091	0.53369
F1	0.30629	0.10066	0.40656
N1	0.93281	0.96897	0.59302
C6	0.39683	0.07653	0.28265
H3	0.35406	0.02268	0.31372
C3	0.62118	0.23076	0.38393
H2	0.61741	0.14332	0.36262
F1	0.40566	0.18849	0.47614
N1	0.84701	0.97728	0.49205
F1	0.31571	0.37089	0.41699
H1	0.98043	0.80112	0.62429
C3	0.53176	0.29523	0.39129
H1	0.82273	0.82119	0.4547
C6	0.4596	0.10392	0.17972
C3	0.53912	0.40743	0.41871
H2	0.47279	0.46021	0.42641
C3	0.63293	0.4548	0.43769
H2	0.63828	0.54306	0.45787
C6	0.40685	0.03675	0.22197
H6	0.37217	0.95946	0.20683
C6	0.49172	0.25195	0.25963
H3	0.52507	0.3364	0.27364
C6	0.50141	0.21262	0.19916
H3	0.54246	0.2659	0.16676
C4	0.43091	0.2379	0.36801
C2	0.82181	0.43717	0.45524
C3	0.71446	0.27676	0.40351
H2	0.78278	0.22521	0.3984
C7	0.47127	0.0629	0.1143
C6	0.44045	0.18424	0.30252
H5	0.89404	0.11814	0.55098
C1	0.85457	0.8595	0.48978
C9	0.89167	0.02202	0.54327
C1	0.93735	0.8515	0.58615
Zn1	0.45239	0.88385	0.01492
O4	0.32239	0.96853	0.97968
O1	0.3928	0.14268	0.96323
F1	0.87204	0.07467	0.82987
O1	0.01008	0.36403	0.57691
F1	0.96591	0.45271	0.91657
C5	0.90117	0.35927	0.91736
C5	0.84437	0.1702	0.8634

O1	0.94352	0.54245	0.59973
F1	0.76047	0.21397	0.83313
C3	0.21896	0.11872	0.93893
N1	0.40404	0.71551	0.03326
F1	0.80584	0.40238	0.90646
N1	0.42812	0.53654	0.09239
C3	0.8987	0.42431	0.7827
H2	0.85729	0.47971	0.81399
C3	0.11993	0.27401	0.88772
H2	0.11657	0.36004	0.86479
F1	0.90529	0.31468	0.97619
N2	0.34396	0.53022	0.99077
F1	0.8162	0.13164	0.91966
H1	0.45986	0.69155	0.12715
C3	0.03131	0.20845	0.89374
H4	0.33327	0.67781	0.9554
C3	0.95977	0.39552	0.67941
C3	0.03803	0.09763	0.92336
H6	0.97113	0.04399	0.92972
C3	0.13089	0.05302	0.94513
H6	0.13564	0.97251	0.96756
C3	0.90835	0.46358	0.72186
H2	0.87427	0.54755	0.70679
C3	0.99184	0.24781	0.75979
H6	0.02554	0.16316	0.77406
C9	0.00165	0.28679	0.69919
H5	0.04233	0.23309	0.66668
C4	0.93054	0.26395	0.86869
C2	0.31909	0.07087	0.96239
C3	0.21245	0.23031	0.91035
H2	0.28054	0.28231	0.90546
C2	0.97163	0.43682	0.61379
C3	0.94074	0.31589	0.80271
H1	0.39351	0.3764	0.03891
C8	0.35271	0.64797	0.98906
C1	0.38649	0.47846	0.04259
C1	0.43538	0.65381	0.08566
Zn1	0.04715	0.38623	0.4849
O1	0.17793	0.46573	0.52016
O2	0.11079	0.64717	0.53674
F1	0.62765	0.59008	0.67646
O3	0.4893	0.865	0.9226
F1	0.53336	0.95645	0.58299
C5	0.59847	0.8636	0.58222
C5	0.65731	0.68056	0.6399

O1	0.5556	0.0377	0.89953
F1	0.73925	0.72967	0.67003
C3	0.28379	0.62027	0.56092
N1	0.09809	0.21937	0.46598
F1	0.69361	0.90582	0.5931
N1	0.07213	0.04011	0.40736
C6	0.60664	0.92446	0.71874
H3	0.65361	0.97587	0.68886
C3	0.38172	0.7776	0.61064
H2	0.38459	0.86452	0.63265
F1	0.59407	0.81772	0.52355
N1	0.15748	0.03412	0.50843
F1	0.68864	0.63501	0.58634
H1	0.04268	0.20546	0.38481
C3	0.47048	0.71183	0.60575
H1	0.17895	0.1821	0.54917
C6	0.53923	0.89746	0.82039
C3	0.46486	0.59975	0.57753
H2	0.53165	0.54577	0.57232
C3	0.37201	0.55429	0.55582
H2	0.36791	0.46686	0.5343
C6	0.59763	0.96161	0.77992
H6	0.63748	0.03432	0.79702
C6	0.49968	0.75699	0.7379
H3	0.46184	0.67602	0.72207
C6	0.4911	0.79363	0.79893
H3	0.44682	0.74231	0.83059
C4	0.56924	0.76992	0.63118
C2	0.18347	0.57358	0.5375
C3	0.2896	0.73291	0.58838
H2	0.22123	0.78472	0.59265
C7	0.52726	0.93841	0.88572
C6	0.55665	0.82224	0.69669
H5	0.11565	0.90062	0.4555
C1	0.14947	0.15194	0.50998
C9	0.11422	0.98832	0.45714
C1	0.06561	0.1576	0.4139

Table S5: Atomic coordinates for HbMOF3:

Zn1	0.55158	0.12345	0.98822
O1	0.67997	0.03756	1.02233

O1	0.60831	-0.1448	1.04083
H3	1.13659	-0.08303	1.17397
O2	0.9942	-0.37014	1.42909
H3	1.0451	-0.45481	1.08767
C5	1.10541	-0.36994	1.08628
C5	1.16534	-0.17013	1.1434
O2	1.06473	-0.55035	1.40565
H3	1.23941	-0.21887	1.17133
C3	0.78387	-0.12132	1.06306
N1	0.60118	0.29385	0.96926
H3	1.19287	-0.40794	1.09827
N1	0.57542	0.47546	0.90888
C7	1.10199	-0.42779	1.2231
H4	1.14352	-0.4844	1.19177
C3	0.88616	-0.27508	1.1133
H2	0.88871	-0.36347	1.13551
H3	1.10061	-0.32342	1.03331
N1	0.65812	0.48487	1.01171
H3	1.19082	-0.13619	1.09048
N2	0.53299	0.29226	0.86962
H1	0.50776	0.33254	0.8295
H1	0.52726	0.20108	0.87172
C3	0.97457	-0.21162	1.11046
N2	0.69562	0.30923	1.0608
H1	0.73331	0.35633	1.0952
H1	0.69411	0.21834	1.0655
C7	1.04269	-0.40234	1.32627
C3	0.96394	-0.10186	1.08205
H2	1.03097	-0.0462	1.07661
C3	0.87168	-0.05715	1.05971
H2	0.86844	0.03241	1.03874
C7	1.0921	-0.46765	1.28333
H4	1.12486	-0.55425	1.29728
C7	1.01183	-0.25753	1.24467
H4	0.97689	-0.17236	1.23021
C7	1.00288	-0.29594	1.30498
H4	0.96246	-0.23872	1.33669
C4	1.07538	-0.2682	1.13592
C2	0.68346	-0.0723	1.04031
C3	0.79437	-0.23226	1.08978
H2	0.72822	-0.29015	1.09296
C6	1.0331	-0.44413	1.39166
C7	1.06229	-0.32128	1.20145
N2	0.61388	0.65326	0.95659
H1	0.64351	0.70737	0.99157

H1	0.58244	0.69966	0.91921
C1	0.64952	0.36706	1.01148
C1	0.61489	0.53309	0.95937
C1	0.57196	0.35866	0.91799
Zn1	-0.04847	0.63653	-0.48626
O1	-0.17686	0.55066	-0.52039
O1	-0.1052	0.36828	-0.53888
H3	-0.63349	0.43005	-0.672
O1	-0.49106	0.14294	-0.92712
H3	-0.54201	0.05828	-0.58571
C5	-0.60229	0.14313	-0.5843
C5	-0.66223	0.34295	-0.64144
O1	-0.5616	-0.03726	-0.90368
H3	-0.73632	0.29421	-0.66937
C3	-0.28078	0.39174	-0.56106
N1	-0.09808	0.80695	-0.4673
H3	-0.68978	0.10515	-0.59631
N1	-0.0723	0.98854	-0.40692
C3	-0.5989	0.0853	-0.72114
H2	-0.64043	0.02869	-0.68981
C3	-0.38307	0.23801	-0.61134
H2	-0.38562	0.14962	-0.63355
H3	-0.59751	0.18966	-0.53135
N1	-0.15503	0.99795	-0.50973
H3	-0.68773	0.3769	-0.58851
N2	-0.0299	0.80534	-0.36765
H1	-0.00466	0.84562	-0.32753
H1	-0.02416	0.71417	-0.36975
C3	-0.47149	0.30146	-0.60848
N2	-0.19253	0.82232	-0.55883
H1	-0.23021	0.86941	-0.59323
H1	-0.19101	0.73144	-0.56354
C3	-0.53962	0.11075	-0.82432
C3	-0.46084	0.41124	-0.5801
H2	-0.52788	0.4669	-0.57465
C3	-0.36857	0.45594	-0.55776
H2	-0.36535	0.5455	-0.53678
C3	-0.58899	0.04543	-0.78136
H2	-0.62176	-0.04116	-0.79531
C3	-0.50868	0.25553	-0.74269
H2	-0.47379	0.34072	-0.72825
C3	-0.49977	0.21713	-0.80301
H2	-0.45939	0.27438	-0.83473
C4	-0.57228	0.24491	-0.63395
C2	-0.18038	0.44079	-0.5383

C3	-0.29127	0.28083	-0.58782
H2	-0.22512	0.22293	-0.59099
C2	-0.53007	0.06894	-0.8897
C3	-0.5592	0.1918	-0.69949
N2	-0.11078	1.16635	-0.45462
H1	-0.14042	1.22045	-0.48961
H1	-0.07933	1.21275	-0.41724
C1	-0.14644	0.88013	-0.5095
C1	-0.1118	1.04616	-0.45742
C1	-0.06887	0.87174	-0.41602
Zn1	-0.55156	-0.12346	-0.98823
O1	-0.67997	-0.03753	-1.02234
O1	-0.60829	0.14479	-1.04085
H3	-1.13659	0.08303	-1.17397
O2	-0.99419	0.37013	-1.42909
H3	-1.0451	0.45481	-1.08767
C5	-1.10539	0.36995	-1.08627
C5	-1.16534	0.17013	-1.1434
O2	-1.06471	0.55035	-1.40564
H3	-1.23942	0.21887	-1.17133
C3	-0.78391	0.12134	-1.06303
N1	-0.60119	-0.29387	-0.96926
H3	-1.19289	0.40795	-1.09828
N1	-0.57542	-0.47546	-0.90888
C7	-1.10201	0.42778	-1.22311
H4	-1.14352	0.48439	-1.19177
C3	-0.88616	0.27506	-1.11331
H2	-0.88871	0.36347	-1.1355
H3	-1.1006	0.32342	-1.03331
N1	-0.65812	-0.48485	-1.01171
H3	-1.19082	0.13618	-1.09048
N2	-0.533	-0.29227	-0.86963
H1	-0.50776	-0.33254	-0.8295
H1	-0.52727	-0.20109	-0.87171
C3	-0.9746	0.21161	-1.11044
N2	-0.69563	-0.30922	-1.0608
H1	-0.7333	-0.35633	-1.0952
H1	-0.69411	-0.21836	-1.0655
C7	-1.04272	0.40235	-1.32628
C3	-0.96393	0.10187	-1.08206
H2	-1.03097	0.04619	-1.07662
C3	-0.87169	0.05715	-1.05972
H2	-0.86844	-0.03241	-1.03874
C7	-1.09208	0.46765	-1.28333
H4	-1.12486	0.55425	-1.29728

C7	-1.01179	0.25755	-1.24465
H4	-0.97688	0.17236	-1.23021
C7	-1.00288	0.29595	-1.30497
H4	-0.96247	0.23871	-1.33669
C4	-1.07536	0.26818	-1.1359
C2	-0.68345	0.07225	-1.04027
C3	-0.79436	0.23226	-1.08981
H2	-0.72822	0.29016	-1.09296
C6	-1.03314	0.44416	-1.39167
C7	-1.06231	0.32128	-1.20145
N2	-0.61388	-0.65326	-0.95659
H1	-0.64351	-0.70737	-0.99157
H1	-0.58243	-0.69967	-0.9192
C1	-0.64953	-0.36706	-1.01147
C1	-0.61487	-0.53307	-0.95938
C1	-0.57198	-0.35862	-0.91799
Zn1	1.05466	0.38966	1.49019
O1	1.18307	0.47554	1.52427
O1	1.1114	0.65789	1.54279
H3	1.63968	0.59612	1.67593
O2	1.49728	0.88324	1.93106
H3	1.5482	0.96789	1.58964
C5	1.60851	0.88304	1.58824
C5	1.66843	0.68322	1.64537
O2	1.56781	1.06345	1.90761
H3	1.74251	0.73195	1.6733
C3	1.28696	0.63438	1.56502
N1	1.10426	0.2192	1.47123
H3	1.69596	0.92102	1.60024
N1	1.07852	0.03763	1.41085
C7	1.60509	0.94087	1.72507
H4	1.64661	0.99748	1.69374
C3	1.38925	0.78817	1.61528
H2	1.3918	0.87656	1.63748
H3	1.6037	0.8365	1.53528
N1	1.16123	0.02821	1.51366
H3	1.69391	0.64928	1.59245
N2	1.03609	0.22082	1.37159
H1	1.01085	0.18055	1.33147
H1	1.03036	0.312	1.37368
C3	1.47769	0.7247	1.61239
N2	1.19872	0.20385	1.56277
H1	1.23641	0.15676	1.59717
H1	1.1972	0.29474	1.56747
C7	1.5458	0.91542	1.82825

C3	1.46705	0.61497	1.58401
H2	1.53407	0.55927	1.57859
C3	1.37476	0.57025	1.5617
H2	1.37153	0.48065	1.54073
C7	1.59518	0.98074	1.7853
H4	1.62796	1.06733	1.79924
C7	1.5149	0.77061	1.74662
H4	1.47998	0.68545	1.73218
C7	1.506	0.80903	1.80695
H4	1.46558	0.75179	1.83866
C4	1.57846	0.78131	1.63789
C2	1.18657	0.58536	1.54229
C3	1.29746	0.74536	1.59174
H2	1.23132	0.80324	1.59493
C6	1.53622	0.95719	1.89363
C7	1.5654	0.83435	1.70341
N2	1.11696	-0.14017	1.45856
H1	1.14661	-0.19429	1.49353
H1	1.08553	-0.18658	1.42117
C1	1.15262	0.14604	1.51344
C1	1.11801	-0.02	1.46135
C1	1.07506	0.15443	1.41994

Table S6: Atomic coordinates of HbMOF4:

Zn1	0.54668	0.11653	0.98511
O3	0.67722	0.03608	0.02031
O1	0.6073	0.86157	0.03636
H3	0.12483	0.91631	0.15382
O1B	0.99971	0.64875	0.42308
H3	0.04338	0.5803	0.08027
C3A	0.09862	0.64658	0.08245
C3A	0.15596	0.83367	0.13835
O1	0.05611	0.46557	0.39935
H3	0.20647	0.77904	0.16603
C2A	0.78099	0.88625	0.06106
N1	0.59549	0.28461	0.96671
H3	0.1751	0.6216	0.09751
N1	0.5699	0.46294	0.90729
C2A	0.10339	0.58266	0.21709
H2	0.14728	0.52959	0.18627
C2A	0.88024	0.73106	0.11193

H2	0.88395	0.64506	0.1349
H3	0.08793	0.66832	0.03427
N2	0.65495	0.47049	0.00875
H3	0.17281	0.88552	0.09759
H1	0.53712	0.29582	0.87643
C2A	0.96874	0.79706	0.10604
H4	0.67434	0.32358	0.04598
C2A	0.04157	0.61178	0.31985
C2A	0.96196	0.90795	0.07666
H6	0.02886	0.96176	0.07058
C2A	0.8689	0.95233	0.05498
H6	0.86395	0.03288	0.03266
C2A	0.09429	0.54418	0.27801
H2	0.12962	0.46159	0.29361
C2A	0.0049	0.75631	0.23885
H6	0.96953	0.83958	0.22393
C6	0.99655	0.71862	0.29974
H5	0.95521	0.77122	0.3323
C3	0.0691	0.74135	0.13126
C2	0.68097	0.93388	0.03749
C2A	0.78763	0.77447	0.08946
H2	0.71955	0.72231	0.0943
C2	0.03181	0.57239	0.38559
C2A	0.05802	0.68887	0.19664
H1	0.62002	0.61194	0.95906
C5	0.64676	0.3525	0.01075
C1	0.61247	0.52155	0.95683
C1	0.56171	0.34585	0.91492
Zn1	0.95665	0.62494	0.51434
O1	0.82727	0.54657	0.47023
O1A	0.89348	0.36306	0.46012
H3	0.36407	0.39595	0.33395
O2	0.50673	0.13746	0.07713
H3	0.43957	0.05922	0.41127
C3A	0.40145	0.14365	0.41742
C3A	0.34397	0.3305	0.36135
O1B	0.44418	0.96289	0.10046
H3	0.27793	0.28152	0.34468
C2A	0.72162	0.38953	0.43076
N1	0.90512	0.79091	0.53369
H3	0.33411	0.09997	0.39779
N1	0.93281	0.96897	0.59302
C3B	0.39683	0.07653	0.28265
H3A	0.35406	0.02268	0.31372
C2A	0.62118	0.23076	0.38393

H2	0.61741	0.14332	0.36262
H3	0.41358	0.19723	0.45876
N1	0.84701	0.97728	0.49205
H3	0.31341	0.36598	0.40346
H1	0.98043	0.80112	0.62429
C2A	0.53176	0.29523	0.39129
H1	0.82273	0.82119	0.4547
C3B	0.4596	0.10392	0.17972
C2A	0.53912	0.40743	0.41871
H2	0.47279	0.46021	0.42641
C2A	0.63293	0.4548	0.43769
H2	0.63828	0.54306	0.45787
C3B	0.40685	0.03675	0.22197
H6	0.37217	0.95946	0.20683
C3B	0.49172	0.25195	0.25963
H3A	0.52507	0.3364	0.27364
C3B	0.50141	0.21262	0.19916
H3A	0.54246	0.2659	0.16676
C3	0.43091	0.2379	0.36801
C2	0.82181	0.43717	0.45524
C2A	0.71446	0.27676	0.40351
H2	0.78278	0.22521	0.3984
C4	0.47127	0.0629	0.1143
C3B	0.44045	0.18424	0.30252
H5	0.89404	0.11814	0.55098
C1	0.85457	0.8595	0.48978
C6	0.89167	0.02202	0.54327
C1	0.93735	0.8515	0.58615
Zn1	0.45239	0.88385	0.01492
O3	0.32239	0.96853	0.97968
O1	0.3928	0.14268	0.96323
H3	0.87286	0.09301	0.83974
O1B	0.01008	0.36403	0.57691
H3	0.95699	0.42959	0.92527
C3A	0.90117	0.35927	0.91736
C3A	0.84437	0.1702	0.8634
O1	0.94352	0.54245	0.59973
H3	0.78275	0.21541	0.83811
C2A	0.21896	0.11872	0.93893
N1	0.40404	0.71551	0.03326
H3	0.82547	0.39379	0.90568
N1	0.42812	0.53654	0.09239
C2A	0.8987	0.42431	0.7827
H2	0.85729	0.47971	0.81399
C2A	0.11993	0.27401	0.88772

H2	0.11657	0.36004	0.86479
H3	0.91257	0.3406	0.96638
N2	0.34396	0.53022	0.99077
H3	0.82207	0.12858	0.90623
H1	0.45986	0.69155	0.12715
C2A	0.03131	0.20845	0.89374
H4	0.33327	0.67781	0.9554
C2A	0.95977	0.39552	0.67941
C2A	0.03803	0.09763	0.92336
H6	0.97113	0.04399	0.92972
C2A	0.13089	0.05302	0.94513
H6	0.13564	0.97251	0.96756
C2A	0.90835	0.46358	0.72186
H2	0.87427	0.54755	0.70679
C2A	0.99184	0.24781	0.75979
H6	0.02554	0.16316	0.77406
C6	0.00165	0.28679	0.69919
H5	0.04233	0.23309	0.66668
C3	0.93054	0.26395	0.86869
C2	0.31909	0.07087	0.96239
C2A	0.21245	0.23031	0.91035
H2	0.28054	0.28231	0.90546
C2	0.97163	0.43682	0.61379
C2A	0.94074	0.31589	0.80271
H1	0.39351	0.3764	0.03891
C5	0.35271	0.64797	0.98906
C1	0.38649	0.47846	0.04259
C1	0.43538	0.65381	0.08566
Zn1	0.04715	0.38623	0.4849
O1	0.17793	0.46573	0.52016
O1A	0.11079	0.64717	0.53674
H3	0.63489	0.61401	0.6735
O2	0.4893	0.865	0.9226
H3	0.55932	0.94867	0.58159
C3A	0.59847	0.8636	0.58222
C3A	0.65731	0.68056	0.6399
O1B	0.5556	0.0377	0.89953
H3	0.7074	0.72113	0.67589
C2A	0.28379	0.62027	0.56092
N1	0.09809	0.21937	0.46598
H3	0.668	0.91388	0.5901
N1	0.07213	0.04011	0.40736
C3B	0.60664	0.92446	0.71874
H3A	0.65361	0.97587	0.68886
C2A	0.38172	0.7776	0.61064

H2	0.38459	0.86452	0.63265
H3	0.58907	0.81798	0.53764
N1	0.15748	0.03412	0.50843
H3	0.67169	0.64869	0.59402
H1	0.04268	0.20546	0.38481
C2A	0.47048	0.71183	0.60575
H1	0.17895	0.1821	0.54917
C3B	0.53923	0.89746	0.82039
C2A	0.46486	0.59975	0.57753
H2	0.53165	0.54577	0.57232
C2A	0.37201	0.55429	0.55582
H2	0.36791	0.46686	0.5343
C3B	0.59763	0.96161	0.77992
H6	0.63748	0.03432	0.79702
C3B	0.49968	0.75699	0.7379
H3A	0.46184	0.67602	0.72207
C3B	0.4911	0.79363	0.79893
H3A	0.44682	0.74231	0.83059
C3	0.56924	0.76992	0.63118
C2	0.18347	0.57358	0.5375
C2A	0.2896	0.73291	0.58838
H2	0.22123	0.78472	0.59265
C4	0.52726	0.93841	0.88572
C3B	0.55665	0.82224	0.69669
H5	0.11565	0.90062	0.4555
C1	0.14947	0.15194	0.50998
C6	0.11422	0.98832	0.45714
C1	0.06561	0.1576	0.4139

2. Comparison of Enthalpy of Adsorption:

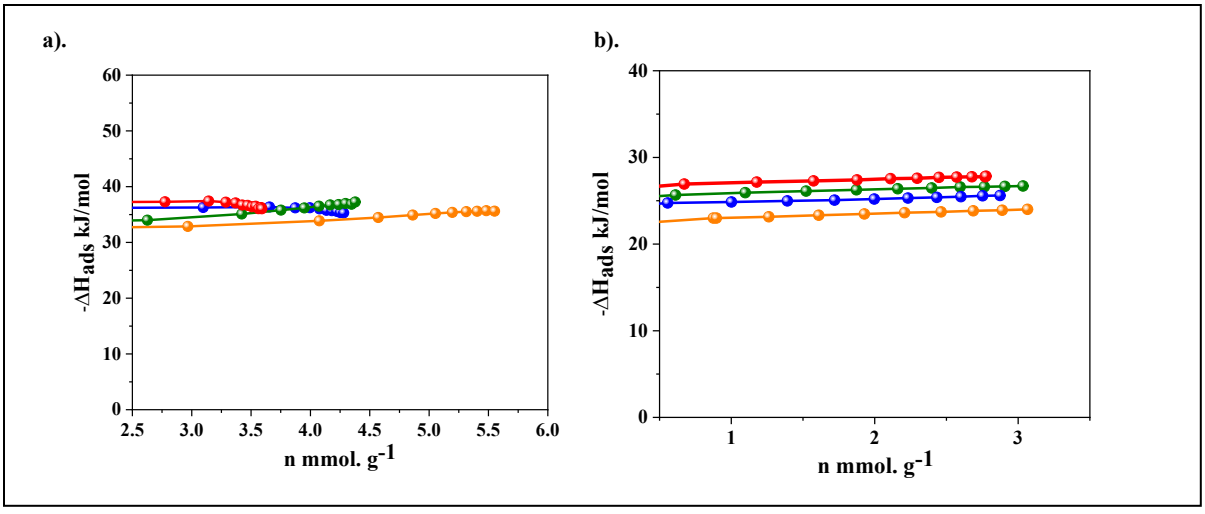


Figure-S4: Comparison of enthalpy on HbMOF series for SO_2 (a) and NO_2 (b) gas at 298K temperature. **(**HbMOF1, Red-sphere; HbMOF2, Green-sphere; HbMOF3, Blue-sphere; HbMOF4, Orange-sphere)

3. Comparison between DFT binding energy and GCMC simulations:

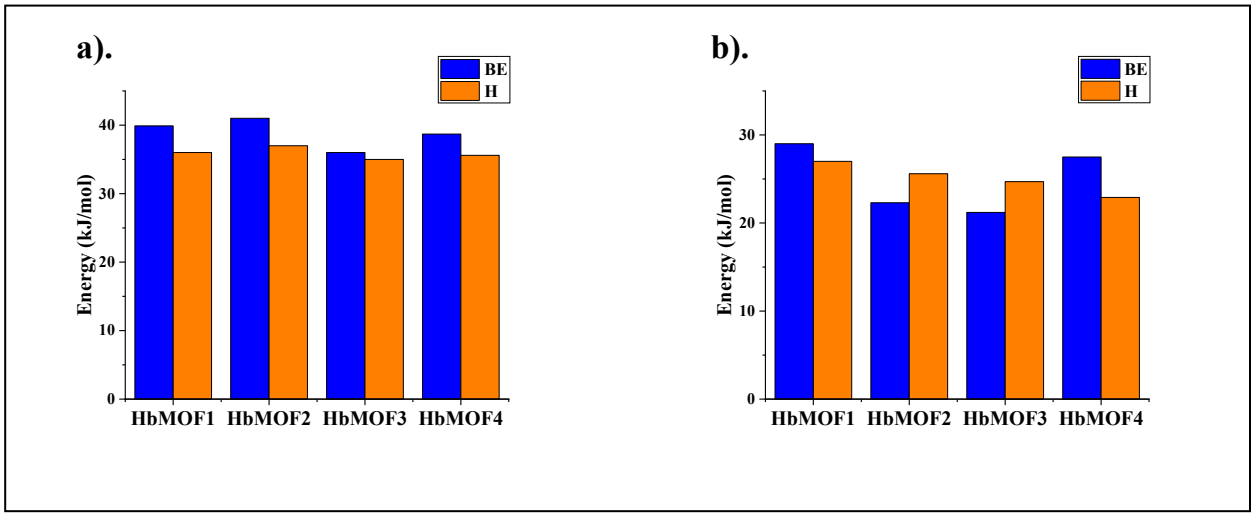


Figure S5: Comparison between the calculated DFT binding energy (BE) with PBE[1-2] functional and GCMC enthalpy of adsorption (H) at 298K for SO_2 (a) and NO_2 (b) in the HbMOF series

4. Comparison of cell parameters:

Table S7: Comparison of cell parameters between DFT optimized and experimental XRD data for HbMOF1.

HbMOF1	**a (Å)**	**b (Å)**	**c (Å)**	**α ( )**	**β ( )**	**γ ( )**
Exp	13.2013	11.2188	21.4127	90	92.970	90
Sim	13.3160	11.2750	21.5640	90	92.970	90

5. Single component isotherm of SO_2 gas at low pressure

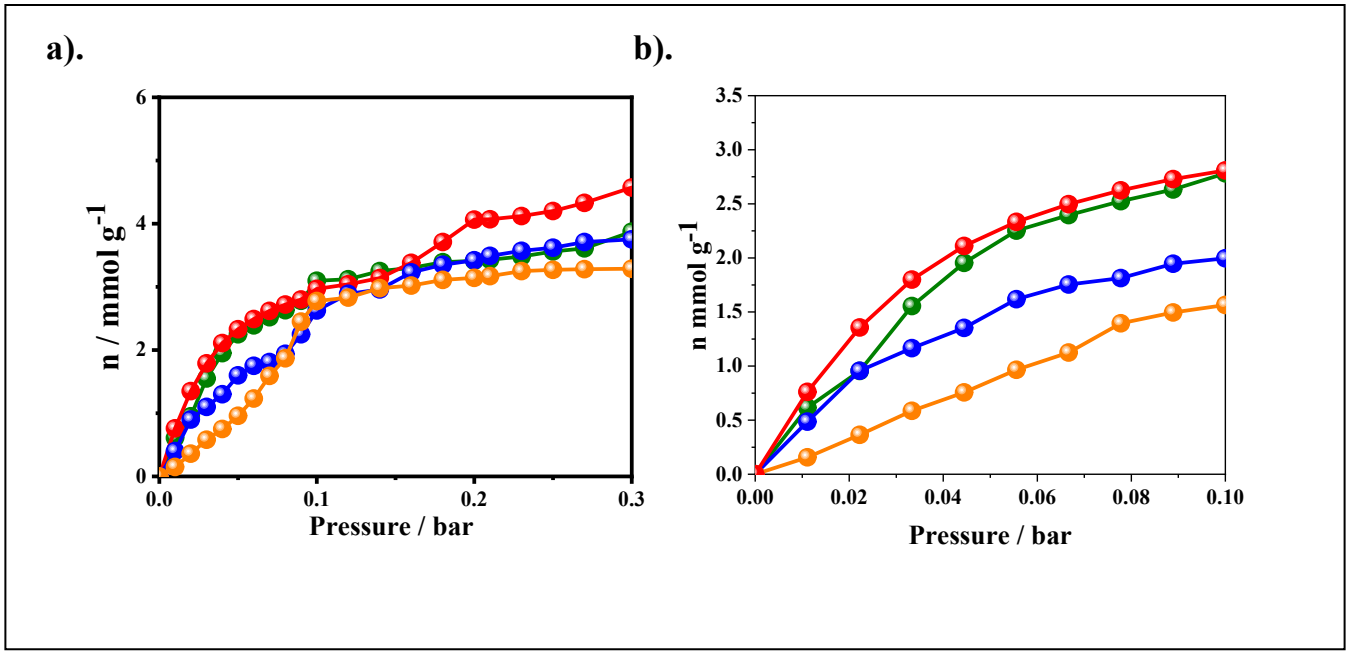


Figure S6: Single component isotherm of SO_2 gas in HbMOF series at 298K and low-pressure a) 0.1-0.3 bar pressure and b) 0-0.1 bar pressure (HbMOF1, Red; HbMOF2, Green; HbMOF3, Blue; HbMOF4, Orange)

6. Theoretical surface area for the HbMOF series:

Table S8: Theoretical surface area for the hypothetical surface area for HbMOF series

Material	Theoretical Surface area (m^2g^{-1})
HbMOF2	261
HbMOF3	247
HbMOF4	230

7. GCMC Trials

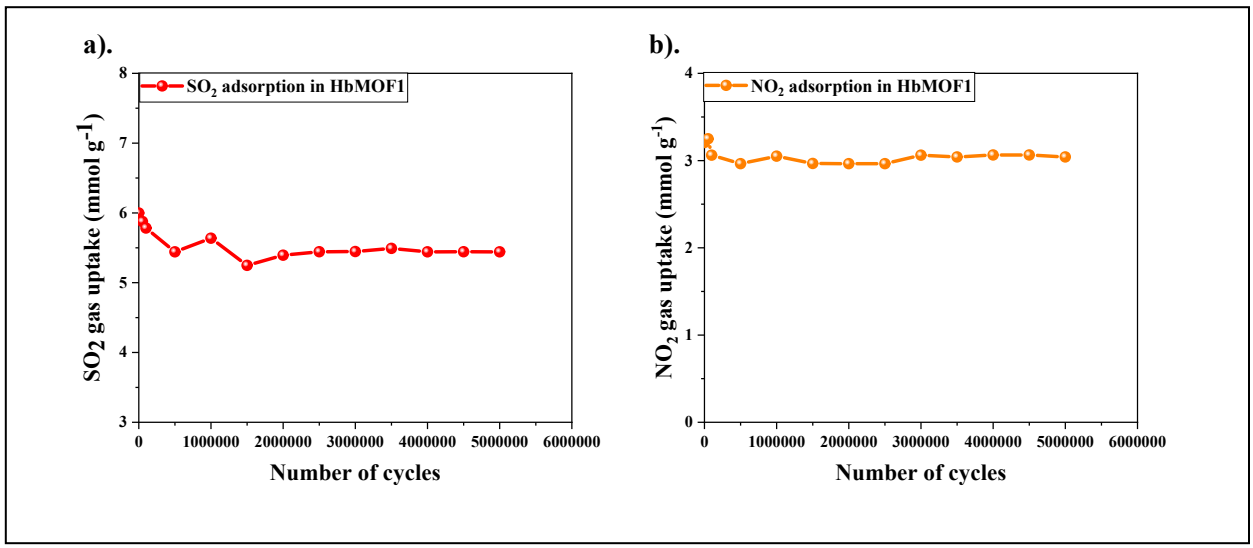


Figure S7: Amount of SO_2 (a) and NO_2 (b) gas adsorbed in each of the initialization cycles in the HbMOF1

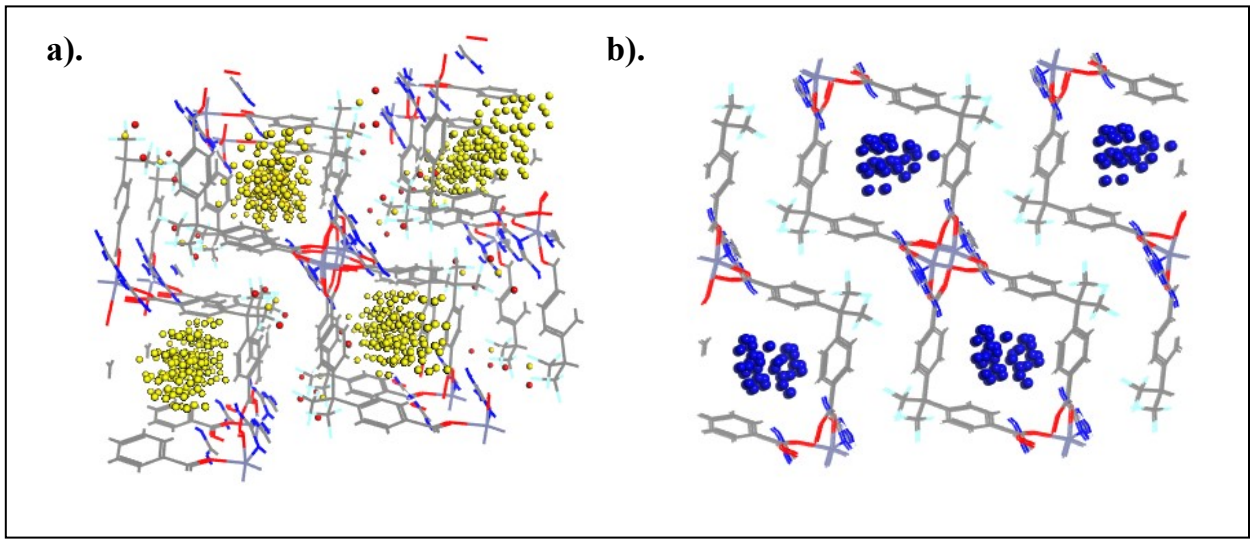


Figure S8: Probabilities of SO_2 (a) and NO_2 (b) gas adsorption of HbMOF1 from the GCMC trials

8. CO_2 gas adsorption on the computationally modelled HbMOFs:

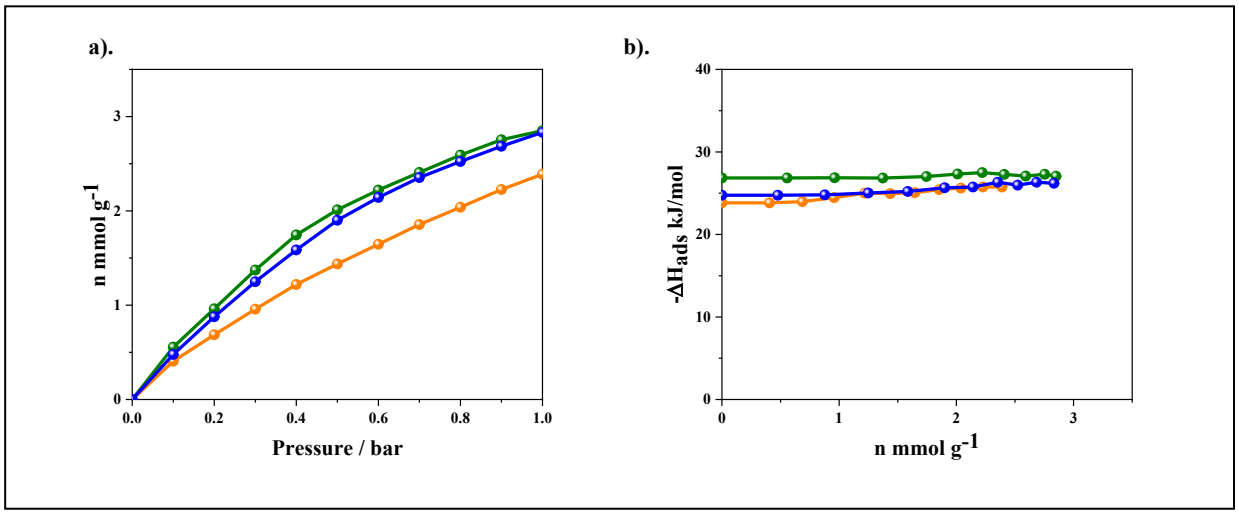
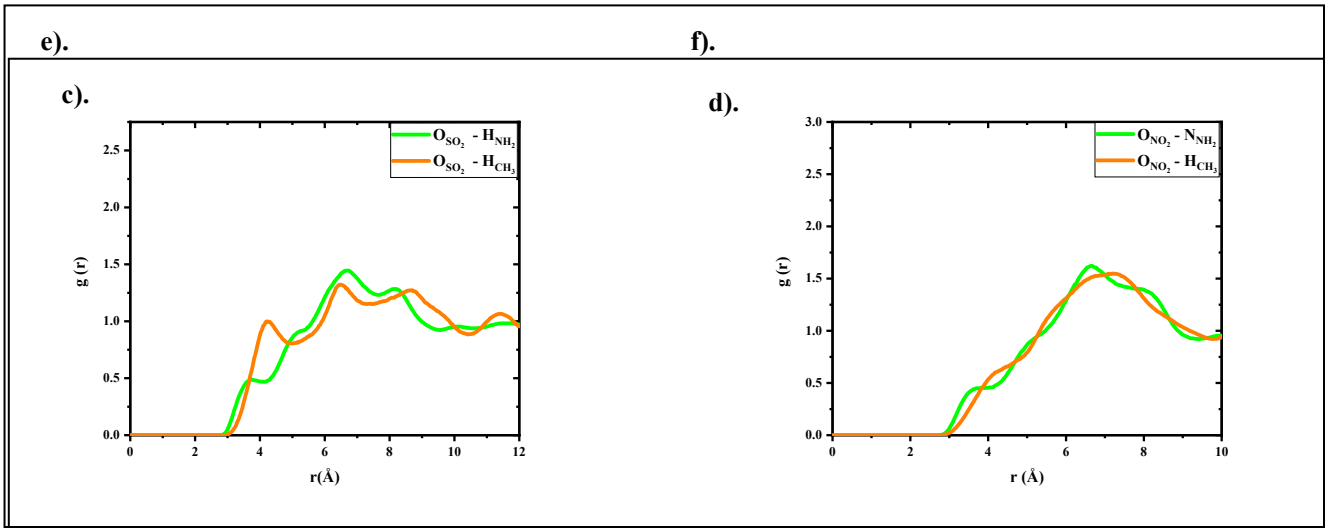


Figure-S9: Simulated CO_2 adsorption isotherm at 298K (a) and heat of enthalpy (b) of HbMOF2, Green-sphere; HbMOF3, Blue sphere; HbMOF4, Orange sphere.

9. Radial Distribution Functions for calculated single component isotherm:



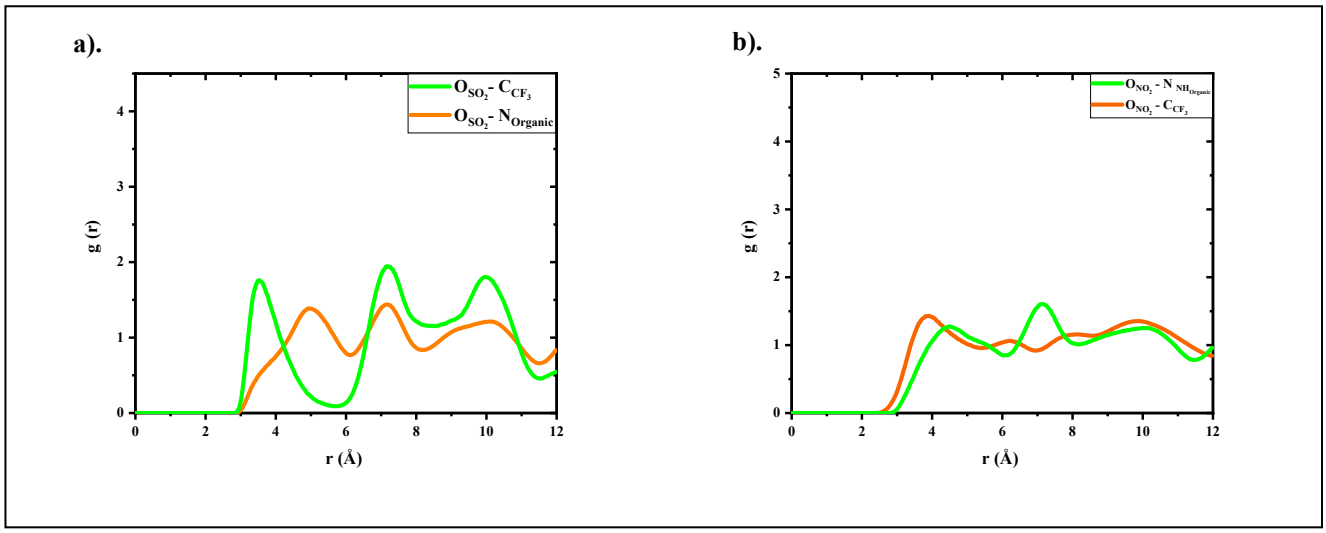


Figure-S10: RDF extracted from the GCMC simulations on SO2 and NO2 on HbMOF series at 1 bar and 298K: HbMOF-2 [(a) – SO_2 , (b) – NO_2] , HbMOF-3 [(c) – SO_2 , (d) – NO_2] and HbMOF-4 [(e) – SO_2 , (f) – NO_2] at 298K temperature.

10. Maps of the occupied positions of SO_2 and NO_2 :

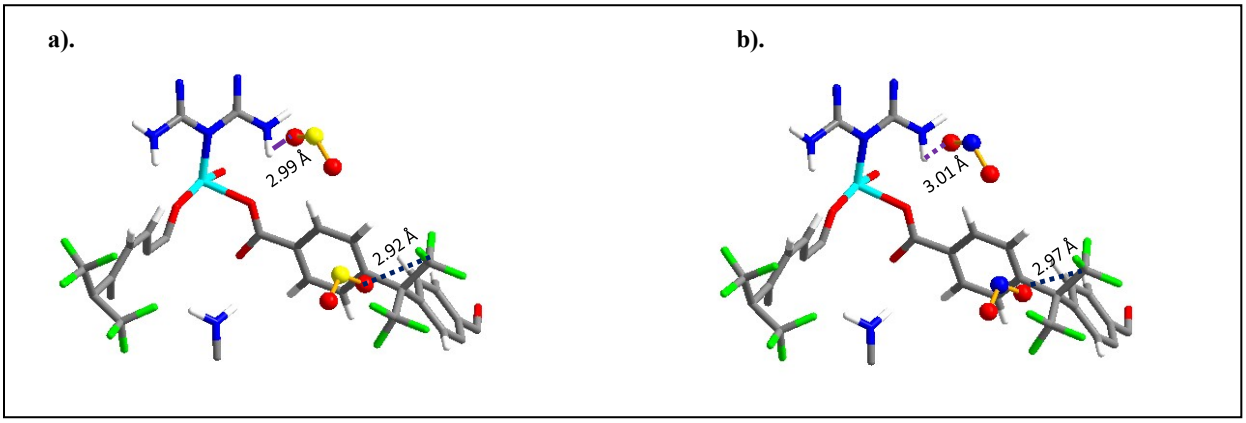


Figure-S11: Local view for the SO_2 (a) and NO_2 (b) interacting distances with functional groups -CF_3 and -NH_2 of HbMOF-1 obtained from the GCMC simulations at 298K and 1 bar.

11. DFT calculation on catalysis using HbMOF-1:

Periodic DFT calculations were carried out in the mixed gaussian plane wave scheme as implemented in the CP2K package with DFT-D3 dispersion corrections. PBE functional was used to calculate the exchange-correlation energy. The triple zeta basis set was considered for Carbon, Nitrogen, Oxygen, Fluorine and Hydrogen whereas the double zeta basis set was considered for Zinc metal. The pseudopotentials that were used in the calculations were derived by Goedecker, Tetter and Hutter. The cut-off energy and basis set for this catalytic fixation were considered from the previous work[15]. The cut-off for the calculation was fixed as 300Ry. The relative energies were computed with the total energy of the corresponding system as mentioned in the eqn.1.

$$E_{relative} = E_{stage} - \left(E_{\mathrm{Hb}MOF} - E_{CO2} - E_{PO}\right) \qquad (1)$$

Where $Estage$, E_{MgMOF}, E_{CO2} and E_{PO} represents the total energies of the HbMOF-1 with each stage of the mechanism. The transition state of the reaction pathway was calculated through the climbing image nudged elastic band method. (CI-NEB).

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