Metal-organic frameworks meet Uni-MOF: a transformer-based gas adsorption detector

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Uni-MOF: A Universal "Gas Adsorption Detector" for MOFs

Table S1. Prediction performance of multi-gas adsorption uptake under varied working conditions. Dataset divided into three splits(train:valid:test = 8:1:1) by material structure.

Regression [coefficient of determination (R^2), higher is better ↑]			
Data Source	hMOF_MOFX-DB	CoRE_MOFX-DB	CoRE_MAP-DB
Gas	CO_2, N_2, CH_4, Kr, Xe	Ar, N_2	CH_4, CO_2, Ar, Kr, Xe, O_2, He
Temperature	273K/298K	77K/87K	150K-300K
Pressure	0.01-10Pa	$1-10^5 Pa$	1Pa-3bar
Property	adsorption uptake (mol/kg)	adsorption uptake (cm^3_{STP}/g)	adsorption uptake (cm^3_{STP}/g)
Data-point	2,477,494	464,824	99,200
Uni-MOF$_{MAP}$	0.9820	0.9158	0.8343

Gas	Critical Temperature (K)	Critical Pressure (MPa)	Acentric Factor	Molecular Mass	Melting point (K)	Boiling point (K)
CH_4	190.8	4.60	0.011	16.0	90.7	111.63
CO_2	304.2	7.38	0.239	44.0	216.5	194.67
Ar	151.2	4.87	0.001	39.9	83.8	87.30
Kr	209.3	5.53	0.005	83.8	115.8	119.70
Xe	289.7	5.84	0.008	131.3	161.3	165.00
O_2	154.6	5.05	0.025	16.0	54.4	90.19
He	2.2	0.23	-0.390	4.0	0.95	4.22
N_2	126.2	3.40	0.039	28.0	63.14	77.36

Table S2. Descriptors of Gas Molecules.

Verification of Experimental Data

MOF	gas	temperature (K)	pressure (Pa)	predictive value (cm^3_{STP}/g)	adsorption uptake (cm^3_{STP}/g)	Reference
Zn2(bdc)2(dabco)	CH_4	393	1	-0.11		
			10	-0.01		
			100	0.10		
			1000	1.23		
			1×10^4	11.74		
			5×10^4	54.03		
			1×10^5	103.44		
			2×10^5	157.63		
			3×10^5	171.88		
			3.5×10^6		175.08	[1]
MIL-101	CH_4	373	1	-0.08		
			10	-0.05		
			100	0.04		
			1000	0.54		
			1×10^4	5.68		
			5×10^4	20.97		
			1×10^5	35.72		
			2×10^5	68.81		
			3×10^5	85.25		
			3.5×10^6		135.86	[1]
Mg-dobdc	CO_2	298	1	0.09		
			10	0.05		
			100	0.07		
			1000	0.44		
			1×10^4	3.13		
			5×10^4	14.13		
			1×10^5	35.5		
			2×10^5	64.06		
			3×10^5	82.25		
			1×10^4		112.05	[2]
			1×10^5		179.28	
Mg-dobdc	CH_4	298	1	0.02		
			10	0.03		
			100	0.03		
			1000	0.17		
			1×10^4	1.62		
			5×10^4	8.02		
			1×10^5	17.72		
			2×10^5	36.91		
			3×10^5	52.34		
			1×10^5		24.93	[2]

Table S3. Experimental Adsorption Uptake Data.

MOF	gas	temperature (K)	pressure (Pa)	predictive value (cm^3_{STP}/g)	adsorption uptake (cm^3_{STP}/g)	Reference
MOF-5	CH_4	298	1	0.04		
			10	0.01		
			100	0.04		
			1000	0.11		
			1×10^4	0.94		
			5×10^4	4.41		
			1×10^5	10.40		
			2×10^5	18.89		
			3×10^5	28.00		
			1×10^5		3.23	3
			3×10^5		4.39	
			5×10^5		9.05	
			9×10^5		16.20	
			1.2×10^6		17.84	
			1.5×10^6		19.59	
			1.86×10^6		21.40	
			2.38×10^6		22.72	
			2.74×10^6		23.02	
			3×10^6		23.28	
MOF-177	CH_4	298	1	-0.01		
			10	0.01		
			100	0.02		
			1000	0.09		
			1×10^4	0.60		
			5×10^4	1.93		
			1×10^5	3.08		
			2×10^5	4.27		
			3×10^5	4.79		
			1×10^5		4.17	3
			4×10^5		7.37	
			7.5×10^5		14.63	
			1.02×10^6		22.16	
			1.3×10^6		25.32	
			1.6×10^6		27.47	
			2.02×10^6		29.11	
			2.21×10^6		29.81	
			2.55×10^6		31.11	
			2.72×10^6		31.40	
			3×10^6		32.63	

Table S4. Experimental Adsorption Uptake Data.

MOF	gas	temperature (K)	pressure (Pa)	predictive value (cm^3_{STP}/g)	adsorption uptake (cm^3_{STP}/g)	Reference
MOF-5	CO_2	296	1	-0.04		
			10	0.01		
			100	0.09		
			1000	0.28		
			1×10^4	1.48		
			5×10^4	7.23		
			1×10^5	14.73		
			2×10^5	32.5		
			3×10^5	49.31		
			1.01×10^5		47.06	[4]
MOF-5	CO_2	298	1	0.05		
			10	0.09		
			100	0.07		
			1000	0.33		
			1×10^4	1.75		
			5×10^4	7.45		
			1×10^5	16.77		
			2×10^5	31.34		
			3×10^5	47.47		
			1.01×10^5		43.03	[5]
			1.01×10^5		41.46	[6]
			1.01×10^5		25.32	[7]
			1.01×10^5		25.10	[8]

Table S5. Experimental Adsorption Uptake Data.

Cross-system forecasting

Table S6. Prediction of adsorption uptake with the division of dataset according to adsorbate gases.

Regression [coefficient of determination (R^2), higher is better ↑]							
Data Source	CoRE_MAP_DB						
Gas in test set	Ar	CH_4	CO_2	Kr	N_2	O_2	Xe
Uni-MOF	0.617	0.465	0.358	0.851	0.449	0.370	0.405

Uni-MOF on single tasks

Table S7. Comparison of Model Performance of argon on CoRE_MOFX-DB. Dataset divided into three splits (train:valid:test = 8:1:1), Uni-MOF$_{single}$ denotes to Uni-MOF model under single working condition's training data, while Uni-MOF$_{mixed}$ indices the mixed mutli-gas absorption model under varied working conditions training in the whole hMOF dataset, that is one vs all performance.

Regression [coefficient of determination (R^2), higher is better ↑]										
Data Source	CoRE_MOFX-DB									
Property	adsorption uptake (cm^3_{STP}/g)									
Gas	Ar									
Temperature	87K									
Pressure (Pa)	0.001	0.01	0.1	1	10	100	1,000	2,000	4,000	6,000
Data-point	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018
Uni-MOF$_{I\&SP}$	0.681	0.677	0.662	0.671	0.725	0.793	0.848	0.839	0.852	0.834
Uni-MOF$_{MAP}$	0.537	0.626	**0.716**	**0.688**	**0.762**	**0.805**	**0.870**	**0.893**	**0.873**	**0.906**
Data Source	CoRE_MOFX-DB									
Property	adsorption uptake (cm^3_{STP}/g)									
Gas	Ar									
Temperature	87K									
Pressure(Pa)	8,000	10,000	12,000	14,000	16,000	18,000	20,000	24,000	28,000	30,000
Data-point	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018
Uni-MOF$_{I\&SP}$	0.899	0.911	0.903	0.923	0.915	0.813	0.916	0.92	0.91	0.904
Uni-MOF$_{MAP}$	0.890	0.903	**0.912**	0.917	**0.930**	**0.930**	**0.930**	**0.929**	**0.930**	**0.927**
Data Source	CoRE_MOFX-DB									
Property	adsorption uptake (cm^3_{STP}/g)									
Gas	Ar									
Temperature	87K									
Pressure (Pa)	32,000	36,000	40,000	50,000	60,000	70,000	80,000	90,000	100,000	
Data-point	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	12,018	
Uni-MOF$_{I\&SP}$	0.912	0.892	0.905	0.91	0.882	0.845	0.847	0.715	0.684	
Uni-MOF$_{MAP}$	**0.929**	**0.928**	**0.928**	0.900	**0.898**	**0.898**	**0.895**	**0.895**	**0.896**	

Table S8. Comparison of Model Performance of nitrogen on CoRE_MOFX-DB. Dataset divided into three splits (train:valid:test = 8:1:1), Uni-MOF$_{single}$ denotes to Uni-MOF model under single working condition's training data, while Uni-MOF$_{mixed}$ indices the mixed mutli-gas absorption model under varied working conditions training in the whole hMOF dataset, that is one vs all performance.

Regression [coefficient of determination (R^2), higher is better ↑]											
Data Source	CoRE_MOFX-DB										
Property	adsorption uptake (cm^3_{STP}/g)										
Gas	N_2										
Temperature	77K										
Pressure (Pa)	1	4	10	18	75	80	200	316	500	1,000	1,334
Data-point	8,388	8,388	3,630	8,356	8,270	3,630	3,596	8,173	3,555	3,504	8,002
Uni-MOF$_{I\&SP}$	0.69	0.734	0.753	0.77	0.852	0.714	0.709	0.876	0.792	0.88	0.779
Uni-MOF$_{MAP}$	**0.782**	**0.795**	**0.789**	**0.828**	0.827	**0.787**	**0.851**	**0.879**	**0.863**	0.853	**0.916**
Data Source	CoRE_MOFX-DB										
Property	adsorption uptake (cm^3_{STP}/g)										
Gas	N_2										
Temperature	77K										
Pressure (Pa)	1,500	2,000	5,000	5,623	20,000	23,714	40,000	60,000	80,000	99,900	100,000
Data-point	3,452	3,389	3,316	7,828	3,247	7,659	3,182	3,130	3,084	3,045	7,478
Uni-MOF$_{I\&SP}$	0.752	0.831	0.86	0.863	0.833	0.878	0.876	0.759	0.731	0.576	0.911
Uni-MOF$_{MAP}$	**0.858**	**0.855**	0.842	**0.934**	**0.911**	**0.942**	**0.879**	**0.871**	**0.868**	**0.869**	0.862

Table S9. Comparison of Model Performance on hMOF absorption. Dataset divided into three splits (train:valid:test = 8:1:1), Uni-MOF$_{single}$ denotes to Uni-MOF model under single working condition's training data, while Uni-MOF$_{mixed}$ indices the mixed mutli-gas absorption model under varied working conditions training in the whole hMOF dataset, that is one vs all performance.

Regression [coefficient of determination (R^2), higher is better ↑]									
Data Source	hMOF_MOFX-DB								
Property	adsorption uptake (mol/kg)								
Gas	CO_2					Kr			N_2
Temperature	298K					273K			298K
Pressure	0.01 bar	0.05 bar	0.1 bar	0.5 bar	2.5 bar	1 bar	5 bar	10 bar	0.09 bar
Data-point	137,652	137,652	137,652	137,652	137,652	137,410	137,652	137,652	137,652
Uni-MOF$_{I\&SP}$	0.839	0.898	0.915	0.941	0.963	0.909	0.947	0.932	**0.847**
Uni-MOF$_{MAP}$	**0.8589**	**0.9158**	**0.9276**	**0.9517**	0.9562	**0.9612**	**0.9686**	**0.9387**	0.8016
Data Source	hMOF_MOFX-DB								
Property	adsorption uptake (mol/kg)								
Gas	CH_4					Xe			N_2
Temperature	298K					273K			298K
Pressure	0.05 bar	0.5 bar	0.9 bar	2.5 bar	4.5 bar	1 bar	5 bar	10 bar	0.9 bar
Data-point	137,652	137,652	137,652	137,652	137,652	137,652	137,652	137,652	137,652
Uni-MOF$_{I\&SP}$	0.862	0.929	0.938	0.954	0.961	0.952	0.970	0.959	0.909
Uni-MOF$_{MAP}$	**0.8648**	**0.9377**	**0.9484**	**0.9656**	**0.9739**	**0.9611**	**0.9759**	**0.9618**	**0.9195**

Table S10. Prediction of intrinsic structural feature for CoRE MOFs and hMOFs. Dataset divided into three splits (train:valid:test = 8:1:1).

Regression [coefficient of determination (R^2), higher is better ↑]								
Data Source	CoRE MOF				hMOF			
Property	PLD (Å)	LCD (Å)	void fraction	volume (cm^3/g)	PLD (Å)	LCD (Å)	void fraction	volume (cm^3/g)
Data-point	12,018	12,018	12,018	12,018	137,953	137,953	137,953	137,953
Uni-MOF$_{I\&SP}$	0.880	0.916	0.936	0.947	0.991	0.991	0.999	0.999

Structure-Property Relationship

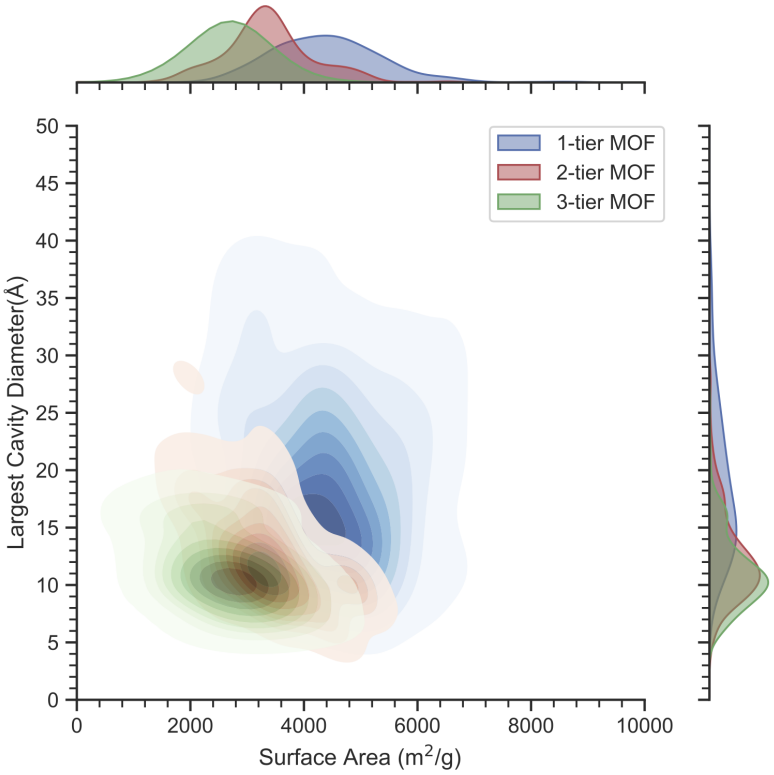

Figure S1. Distribution of surface area and LCD for three tiers within top 10% of MOFs according to their adsorption performance on argon.

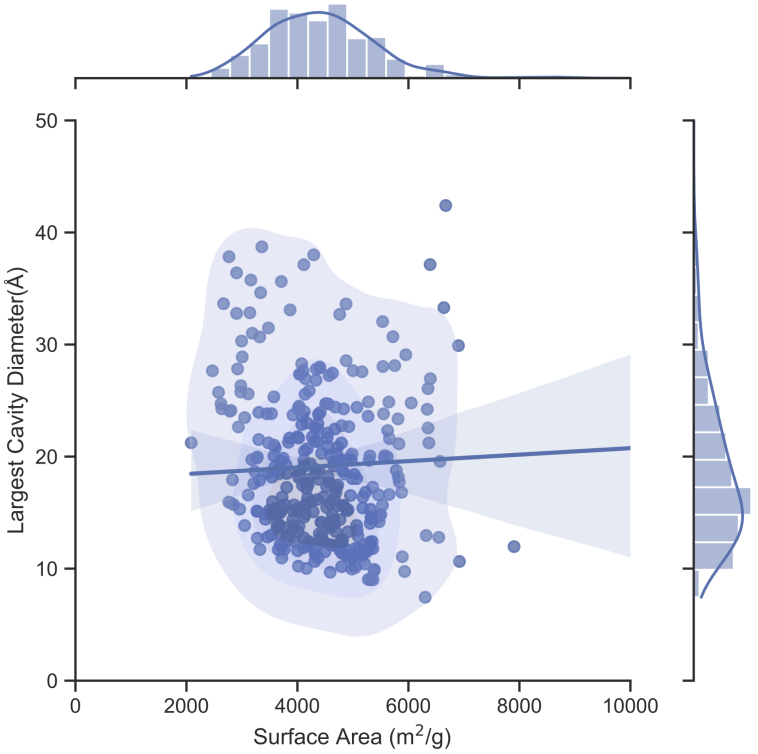

Figure S2. The detailed analysis of surface area and LCD distribution of top tier MOFs for argon.

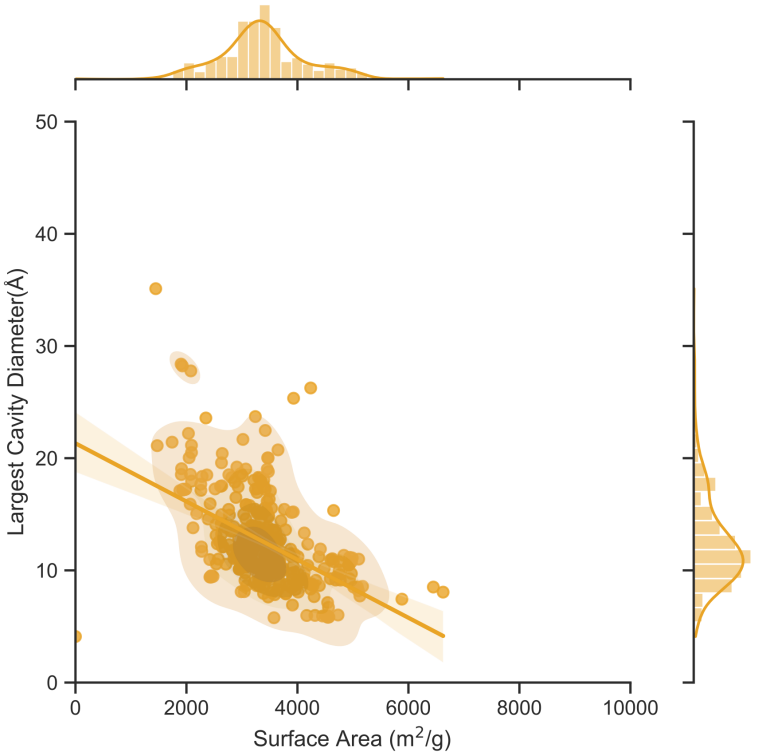

Figure S3. The detailed analysis of surface area and LCD distribution of second tier MOFs for argon.

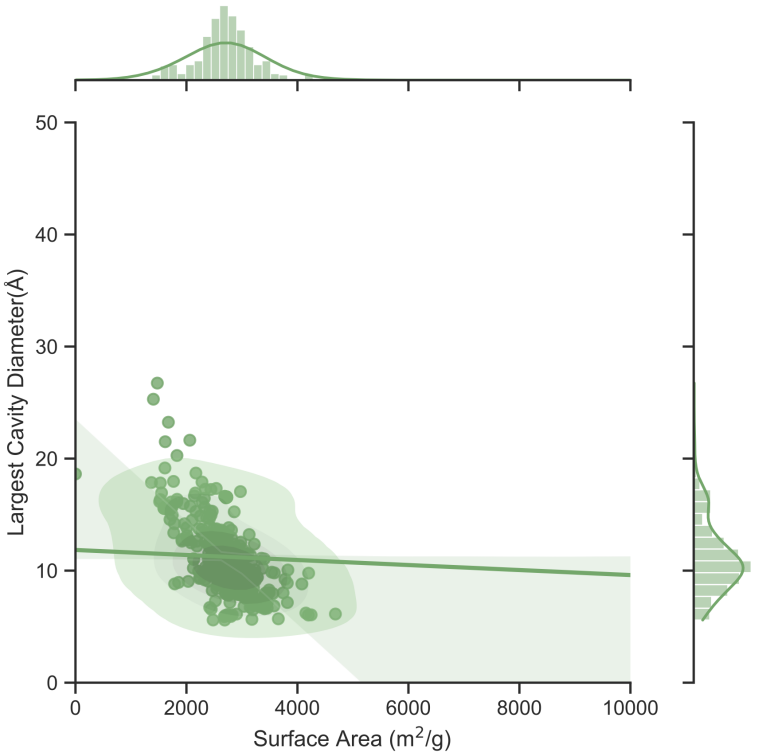

Figure S4. The detailed analysis of surface area and LCD distribution of bottom tier MOFs for argon.

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