

Electronic Supplementary Material

**A Large-Scale Screening of Metal-Organic Frameworks for Iodine Capture  
Combining Molecular Simulation and Machine Learning**

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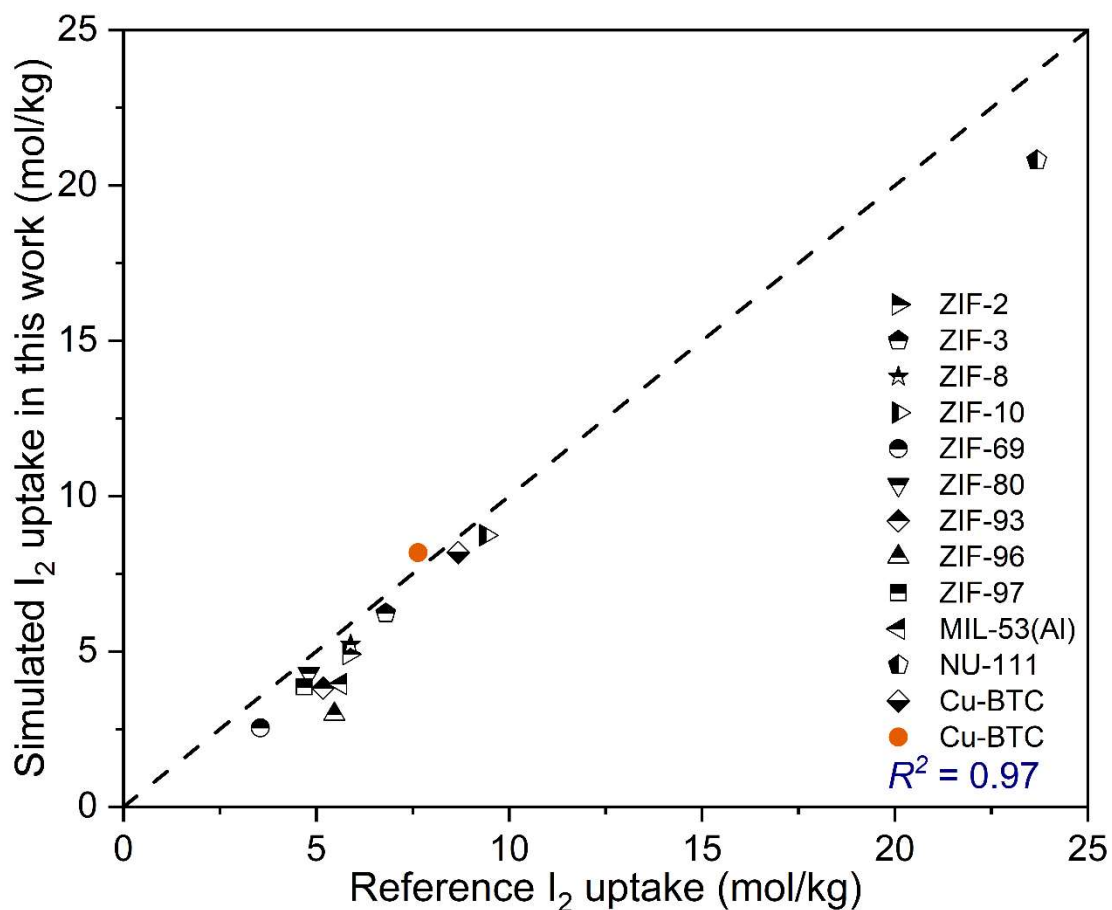
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**Table S1.** LJ potential parameters of MOF framework atoms<sup>1</sup>

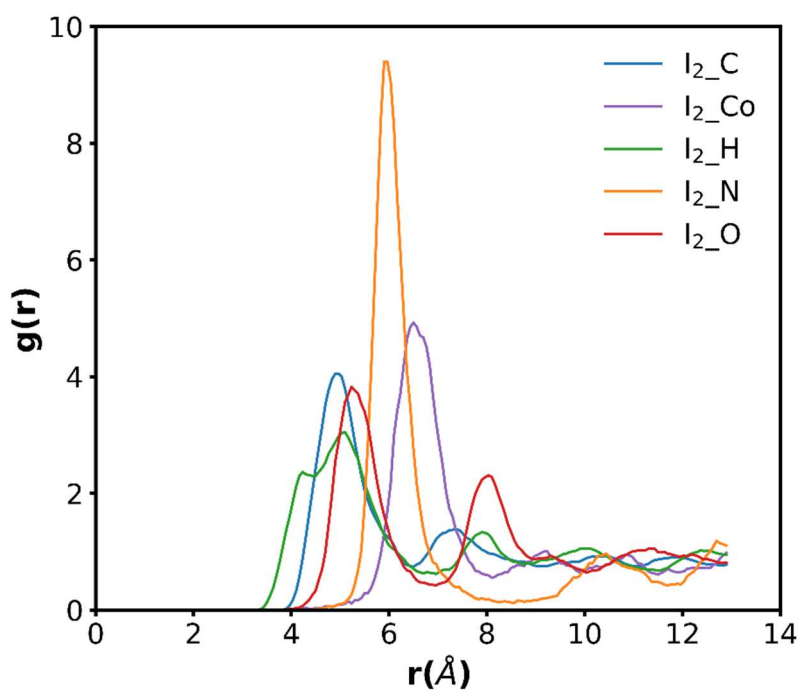
<b>Atom</b>	$\epsilon/k_B(\text{K})$	$\sigma(\text{\AA})$	<b>Atom</b>	$\epsilon/k_B(\text{K})$	$\sigma(\text{\AA})$	<b>Atom</b>	$\epsilon/k_B(\text{K})$	$\sigma(\text{\AA})$
<b>Ac</b>	16.6	3.1	<b>Ge</b>	190.69	3.81	<b>Po</b>	163.52	4.2
<b>Ag</b>	18.11	2.8	<b>Gd</b>	4.53	3	<b>Pr</b>	5.03	3.21
<b>Al</b>	254.09	4.01	<b>H</b>	22.14	2.57	<b>Pt</b>	40.25	2.45
<b>Am</b>	7.04	3.01	<b>Hf</b>	36.23	2.8	<b>Pu</b>	8.05	3.05
<b>Ar</b>	93.08	3.45	<b>Hg</b>	193.71	2.41	<b>Ra</b>	203.27	3.28
<b>As</b>	155.47	3.77	<b>Ho</b>	3.52	3.04	<b>Rb</b>	20.13	3.67
<b>At</b>	142.89	4.23	<b>I</b>	170.57	4.01	<b>Re</b>	33.21	2.63
<b>Au</b>	19.62	2.93	<b>In</b>	301.39	3.98	<b>Rh</b>	26.67	2.61
<b>B</b>	90.57	3.64	<b>Ir</b>	36.73	2.53	<b>Rn</b>	124.78	4.25
<b>Ba</b>	183.15	3.3	<b>K</b>	17.61	3.4	<b>Ru</b>	28.18	2.64
<b>Be</b>	42.77	2.45	<b>Kr</b>	110.69	3.69	<b>S</b>	137.86	3.59
<b>Bi</b>	260.63	3.89	<b>La</b>	8.55	3.14	<b>Sb</b>	225.91	3.94
<b>Bk</b>	6.54	2.97	<b>Li</b>	12.58	2.18	<b>Sc</b>	9.56	2.94
<b>Br</b>	126.29	3.73	<b>Lu</b>	20.63	3.24	<b>Se</b>	146.42	3.75
<b>C</b>	52.83	3.43	<b>Lr</b>	5.53	2.88	<b>Si</b>	202.27	3.83
<b>Ca</b>	119.75	3.03	<b>Md</b>	5.53	2.92	<b>Sm</b>	4.03	3.14
<b>Cd</b>	114.72	2.54	<b>Mg</b>	55.85	2.69	<b>Sn</b>	285.28	3.91
<b>Ce</b>	6.54	3.17	<b>Mn</b>	6.54	2.64	<b>Sr</b>	118.24	3.24
<b>Cf</b>	6.54	2.95	<b>Mo</b>	28.18	2.72	<b>Ta</b>	40.75	2.82
<b>Cl</b>	114.21	3.52	<b>N</b>	34.72	3.26	<b>Tb</b>	3.52	3.07
<b>Cm</b>	6.54	2.96	<b>Na</b>	15.09	2.66	<b>Tc</b>	24.15	2.67
<b>Co</b>	7.04	2.56	<b>Ne</b>	21.13	2.66	<b>Te</b>	200.25	3.98
<b>Cr</b>	7.55	2.69	<b>Nb</b>	29.69	2.82	<b>Th</b>	13.08	3.03
<b>Cu</b>	2.52	3.11	<b>Nd</b>	5.03	3.18	<b>Ti</b>	8.55	2.83
<b>Cs</b>	22.64	4.02	<b>No</b>	5.53	2.89	<b>Tl</b>	342.14	3.87
<b>Dy</b>	3.52	3.05	<b>Ni</b>	7.55	2.52	<b>Tm</b>	3.02	3.01
<b>Eu</b>	4.03	3.11	<b>Np</b>	9.56	3.05	<b>U</b>	11.07	3.02
<b>Er</b>	3.52	3.02	<b>O</b>	30.19	3.12	<b>V</b>	8.05	2.8
<b>Es</b>	6.04	2.94	<b>Os</b>	18.62	2.78	<b>W</b>	33.71	2.73
<b>F</b>	25.16	3	<b>P</b>	153.46	3.69	<b>Xe</b>	229.8	3.97
<b>Fe</b>	6.54	2.59	<b>Pa</b>	11.07	3.05	<b>Y</b>	36.23	2.98
<b>Fm</b>	6.04	2.93	<b>Pb</b>	333.59	3.83	<b>Yb</b>	114.72	2.99
<b>Fr</b>	25.16	4.37	<b>Pd</b>	24.15	2.58	<b>Zn</b>	62.39	2.46
<b>Ga</b>	208.81	3.9	<b>Pm</b>	4.53	3.16	<b>Zr</b>	34.72	2.78

**Table S2.** LJ potential and structural parameters of iodine molecule<sup>2</sup>

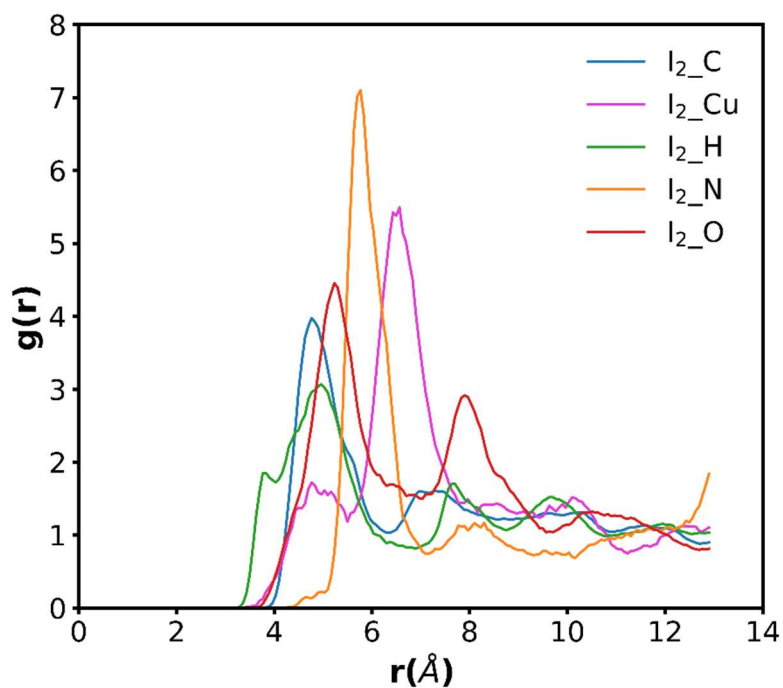
Molecule	Atom	LJ parameters		Molecular model			
		$\epsilon/k_B(\text{K})$	$\sigma(\text{\AA})$	x	y	z	Charge
I <sub>2</sub>	I <sub>2</sub>	550.0	4.982	0.0	0.0	0.0	0.0



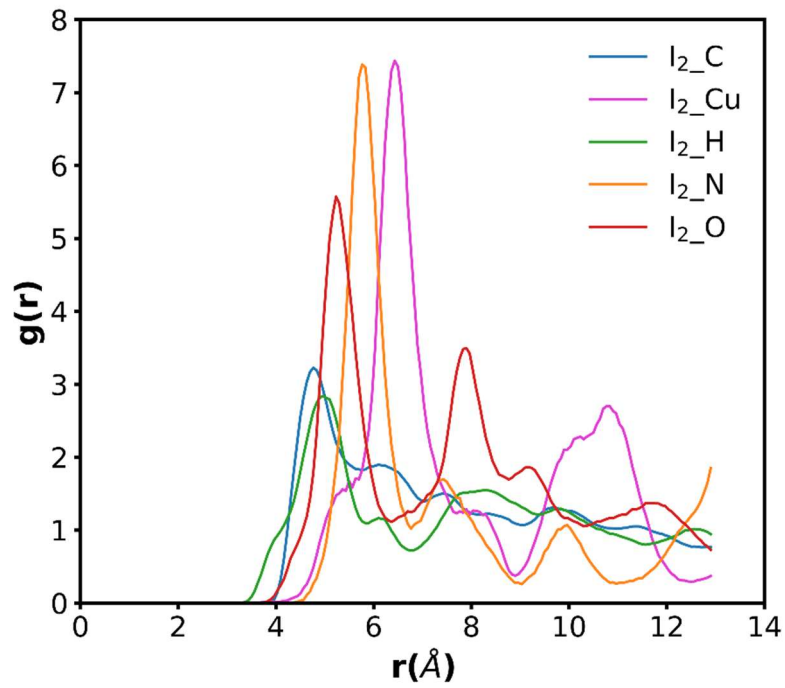
**Fig. S1** Validation of the GCMC results with I<sub>2</sub> uptake values from literature<sup>3, 4</sup> (for Cu-BTC, the orange dot represents an experimental uptake value from literature and the black/white rhombus a computational uptake value from literature).



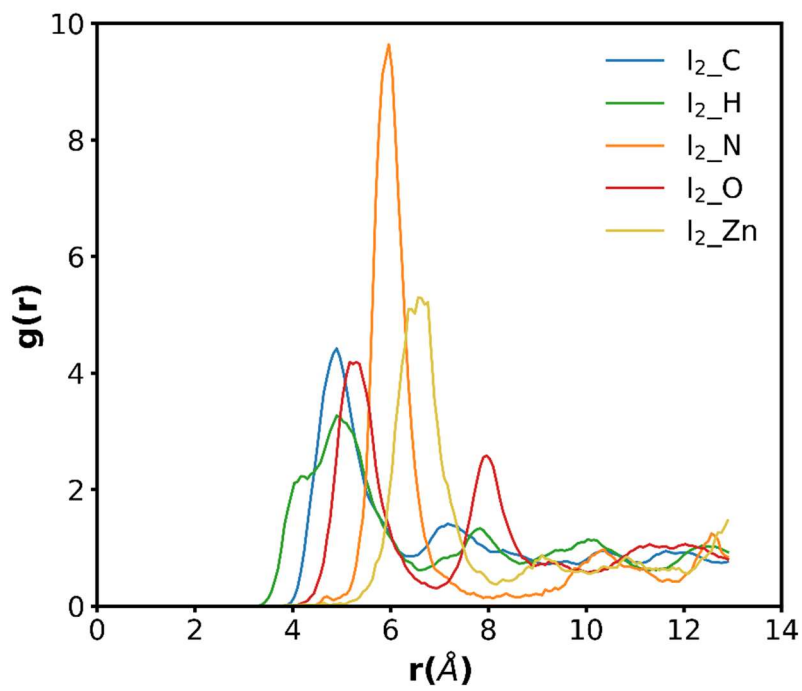
**Fig. S2** The radial distribution function of different atom pairs between the framework atoms of ACODAZ and I<sub>2</sub>.



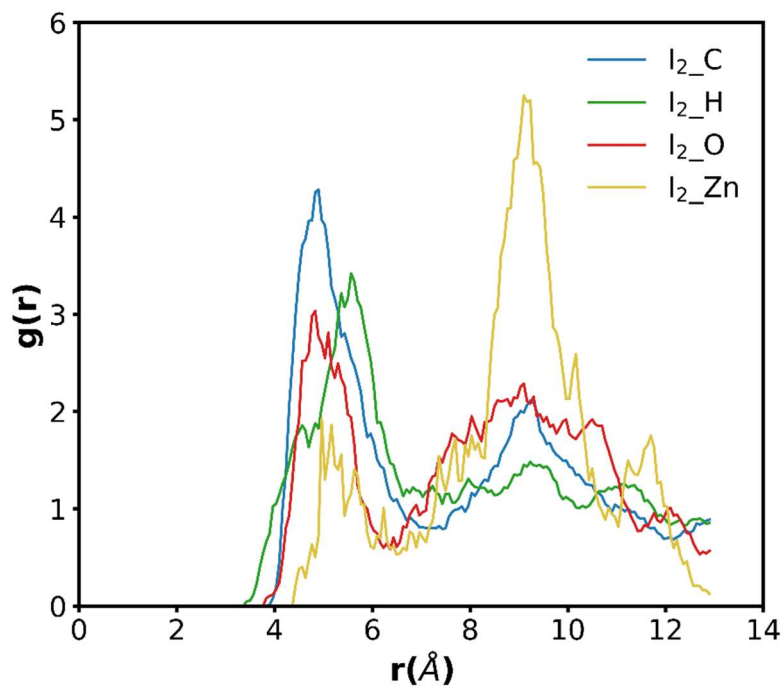
**Fig. S3** The radial distribution function of different atom pairs between the framework atoms of XAFFUH and I<sub>2</sub>.



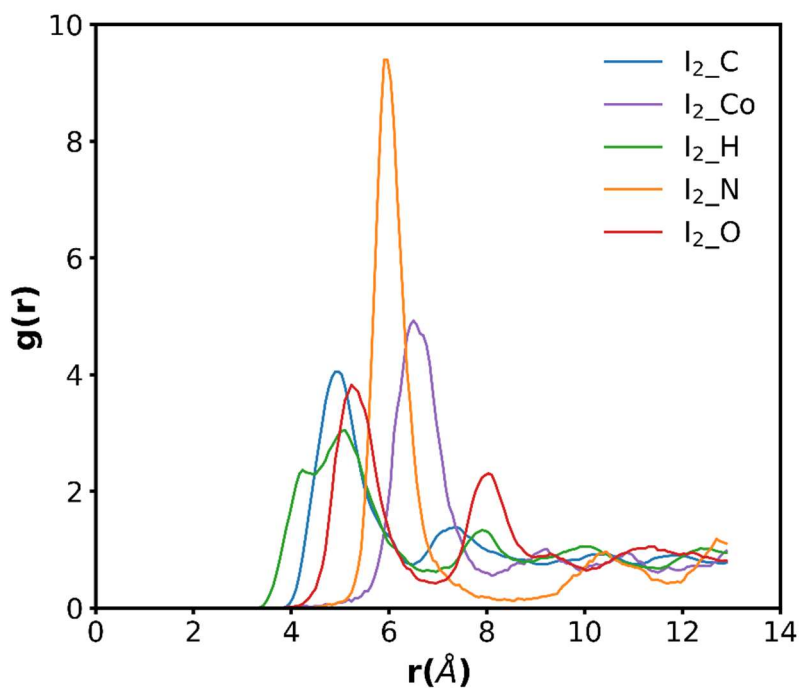
**Fig. S4** The radial distribution function of different atom pairs between the framework atoms of ACOCOM and  $I_2$ .



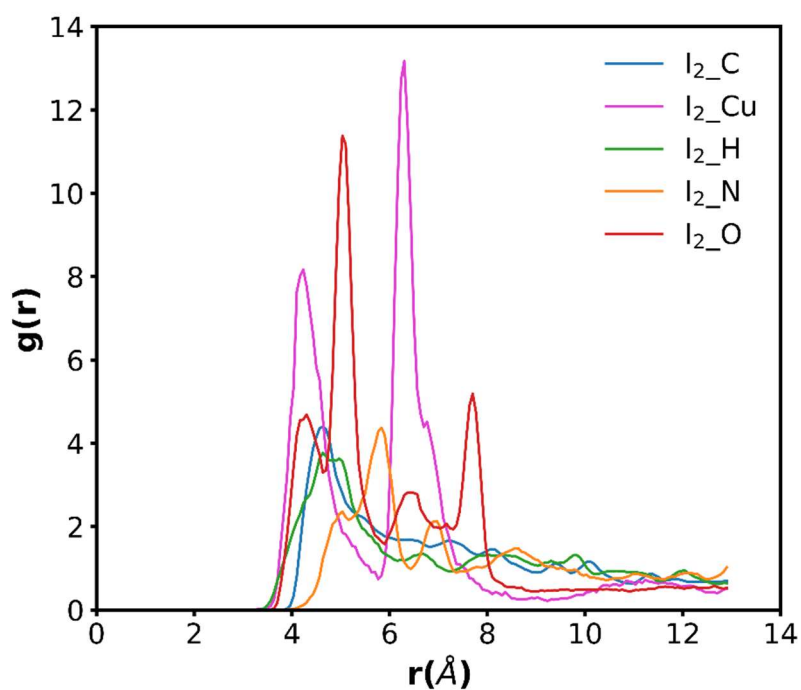
**Fig. S5** The radial distribution function of different atom pairs between the framework atoms of ACOCUS and  $I_2$ .



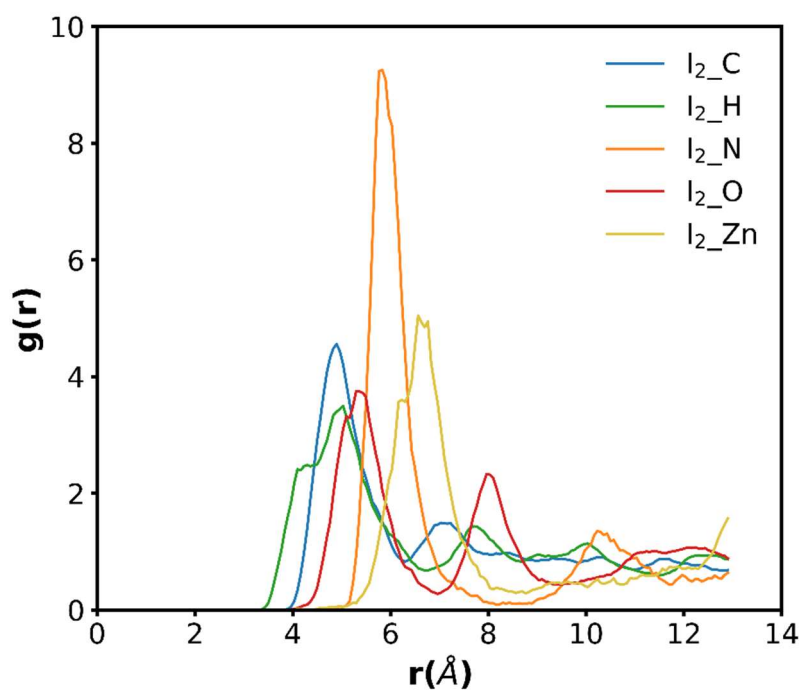
**Fig. S6** The radial distribution function of different atom pairs between the framework atoms of LEJCEK and I<sub>2</sub>.



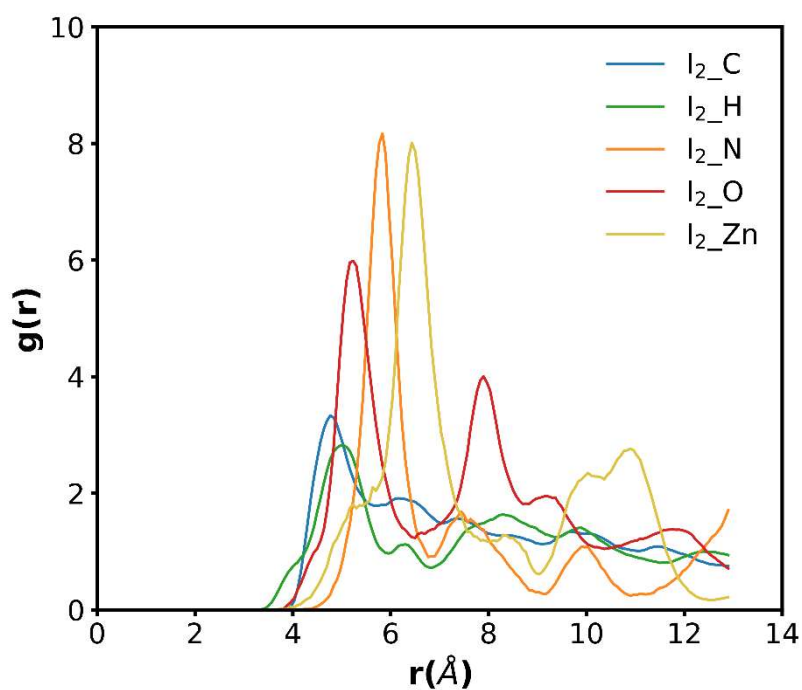
**Fig. S7** The radial distribution function of different atom pairs between the framework atoms of XAFFIV and I<sub>2</sub>.



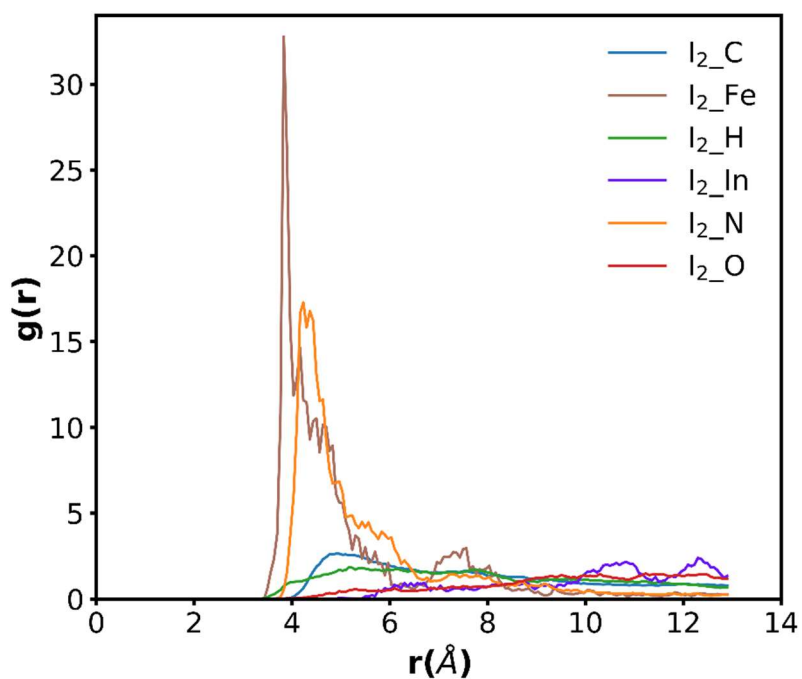
**Fig. S8** The radial distribution function of different atom pairs between the framework atoms of VAGMEX and I<sub>2</sub>.



**Fig. S9** The radial distribution function of different atom pairs between the framework atoms of NATKIF and I<sub>2</sub>.



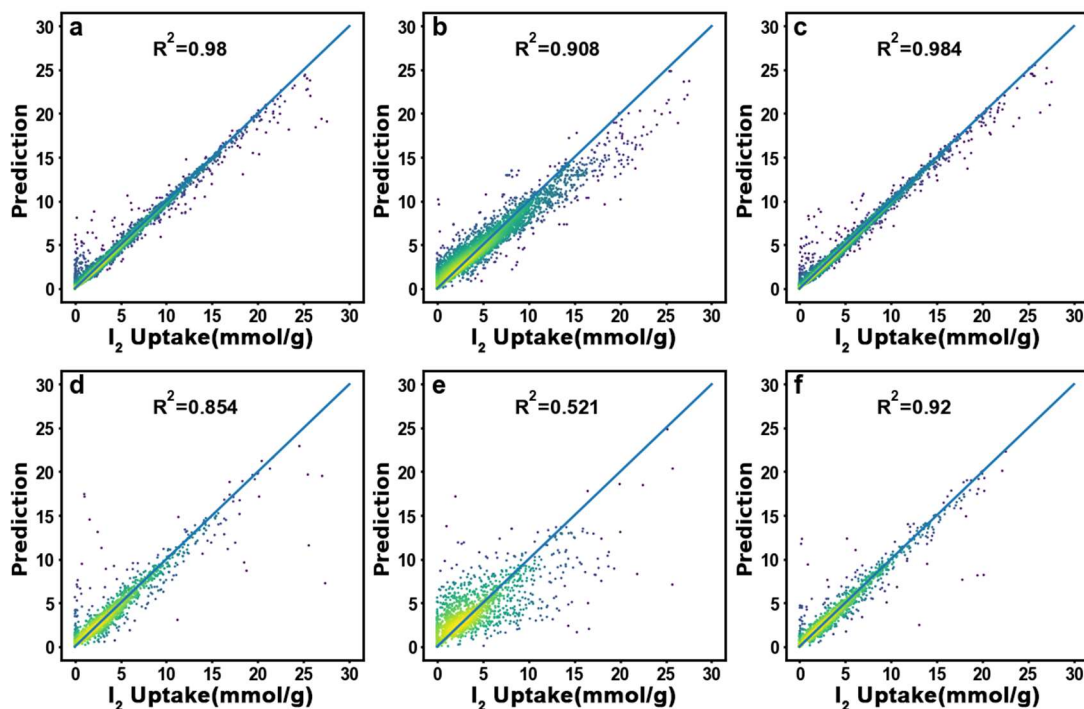
**Fig. S10** The radial distribution function of different atom pairs between the framework atoms of XAFFER and I<sub>2</sub>.



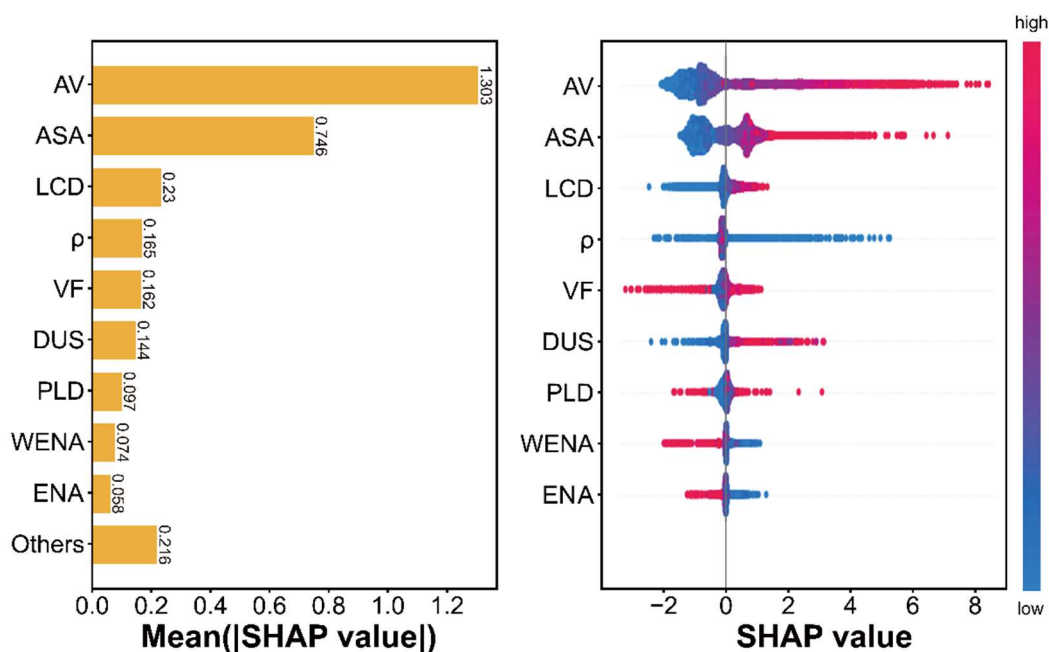
**Fig. S11** The radial distribution function of different atom pairs between the framework atoms of AWUPAL and I<sub>2</sub>.

**Table S3.** Pearson coefficients (R) of all chemical features (Counts of atoms of specific elements; DUS: total degree of unsaturation; MP: metallic percentage; OMR: oxygen-to-metal ratio; ENA: electronegative per atom; WENA: weighted electronegativity per atom; N2O: nitrogen to oxygen ratio).

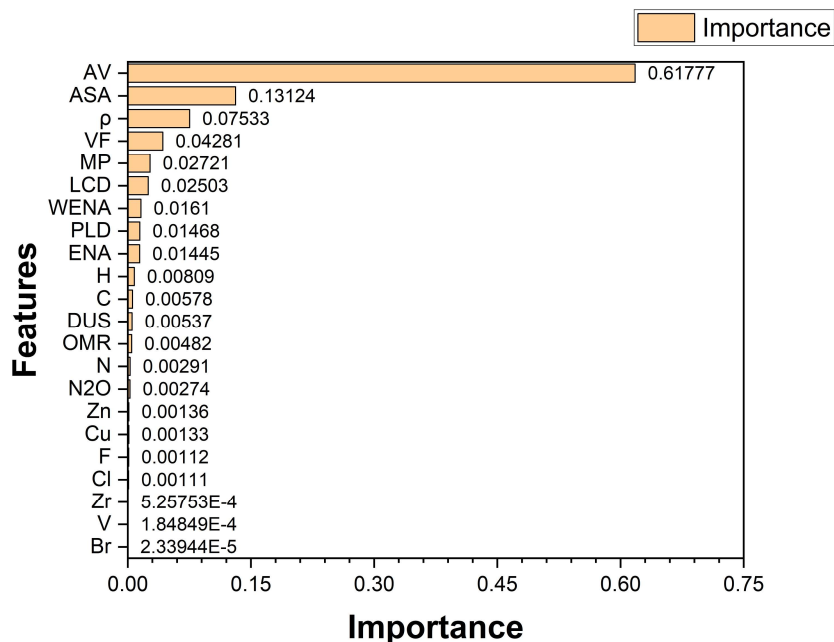
Chemical Features	Pearson R	Chemical Features	Pearson R
H Counts	0.200	DUS	0.322
C Counts	0.294	MP	-0.130
N Counts	0.032	OMR	-0.008
F Counts	0.010	ENA	-0.286
Cl Counts	-0.012	WENA	-0.278
Br Counts	-0.016	N2O	-0.036
V Counts	0.001	Zn Counts	0.006
Cu Counts	0.006	Zr Counts	0.007



**Fig. S12** Visualization of the performance of the pre-trained RF models based on different sets of features (a, d: geometric features only; b, e: chemical features only; c, f: geometric and chemical features both; top row (a-c): train set performance; bottom row (d-f): test set performance).



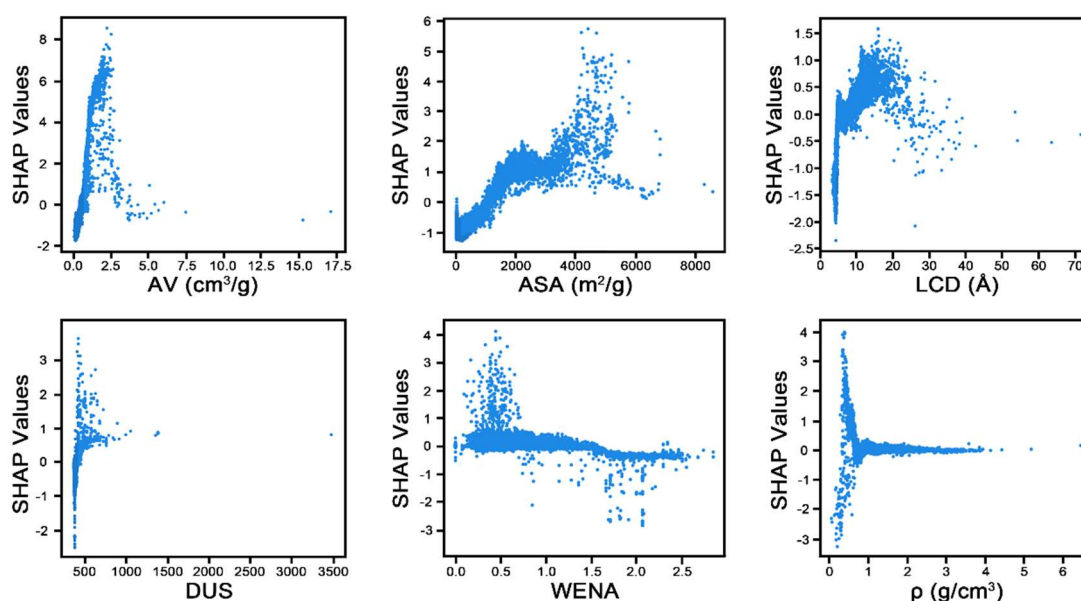
**Fig. S13** Left: mean absolute SHAP values of selected features in the pre-trained RF model; right: beeswarm plot of SHAP values for top nine features in importance, with actual feature values normalized and color-coded (higher: more red; lower: more blue).



**Fig. S14** Importance values of all features generated by the pre-trained RF model.

**Table S4.** Hyperparameter tuning space and optimal hyperparameters

Hyperparameters	Spaces	Optimal		
		Geometric	Chemical	Both
Number of Trees	75, 100, 125, 150, 175, 200	100	200	175
Max Depth	8, 16, 32, 64, 128	32	128	64
Min Samples Leaf	2, 4, 6, 8, 16	2	2	2
Criterion	<i>Squared, Absolute, Poisson</i>	<i>Squared</i>	<i>Squared</i>	<i>Squared</i>

**Fig. S15** Scatter plots for the top 6 important features from SHAP analysis.

**Table S5.** Comparison of performances ( $R^2$ ) for the random forest (RF), support vector machine (SVM), artificial neural network (ANN) models. All of these models were trained on the same train set and tested their performances on the same test set.

Features	RF	SVM	ANN
Geometric	0.879	0.770	0.708
Chemical	0.539	0.211	0.276
Both	0.926	0.814	0.758

## Reference

1. Rappe A K, Casewit C J, Colwell K S, Goddard W A, Skiff W M (1992). UFF, a full periodic table force field for molecular mechanics and molecular dynamics simulations. *Journal of the American Chemical Society*, 114(25): 10024-10035
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3. Zhang X, Maddock J, Nenoff T M, Denecke M A, Yang S, Schröder M (2022). Adsorption of iodine in metal–organic framework materials. *Chemical Society Reviews*, 51(8): 3243-3262
4. Xie W, Cui D, Zhang S-R, Xu Y-H, Jiang D-L (2019). Iodine capture in porous organic polymers and metal–organic frameworks materials. *Materials Horizons*, 6(8): 1571-1595