Supporting Information

Iodine capture of two-dimensional layered uranyl-organic framework: A combined DFT and AIMD study

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Table S1. The Cartesian coordinates of optimized structures for cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.10384670	15.70164184	3.75622923
O	43.35867208	15.73579128	5.53657113
O	43.00306901	15.64260441	1.97669866
O	42.93292120	13.18676797	3.81366768
O	45.01568408	13.92742021	3.76606752
C	44.16337345	12.96789627	3.82731891
H	44.54717583	11.91444945	3.89280798
O	41.19615404	17.14051210	3.91312211
O	40.83743079	14.96906041	4.00837040
N	32.51036804	17.17116051	4.69329522
N	33.72478122	15.10231076	4.67200271
N	31.33581361	15.08833412	4.89782261
N	30.16616443	17.05053148	4.91644438
H	29.41615264	16.36341107	5.01691556
N	34.78478079	17.20070538	4.48085165
H	34.56170040	18.19821762	4.45914932
N	32.62133611	13.11164621	4.86629111
H	33.59227514	12.80174741	4.78740750
H	28.38900496	22.07506314	4.84460348
C	28.77156057	21.04390616	4.85784164
C	28.37741543	18.64889588	5.00611690
H	27.67877228	17.80277845	5.10972513
C	30.65319193	19.48435079	4.75774638
H	31.72594639	19.28257756	4.66834084
C	27.88915417	19.95929805	4.98974038
H	26.80608574	20.13234173	5.08110703
C	30.14713761	20.79159350	4.74308460
H	30.85137979	21.63143904	4.63876969
C	29.76495965	18.39333687	4.89049455
C	31.39374882	16.44429461	4.83024672
C	32.52458042	14.47871206	4.81347777
C	33.64997591	16.43609245	4.61974739
C	31.66504207	12.09629967	5.00538014
C	31.25866551	9.68951618	5.15182740
H	31.65458679	8.66262827	5.15761729
C	30.27670839	12.32671500	5.13297614
H	29.91119821	13.35912091	5.12346497
C	32.14341479	10.76403717	5.01655889
H	33.22496717	10.57709342	4.91701496

C	29.40369584	11.23815965	5.26775318
H	28.32454547	11.43301515	5.36626891
C	29.87871248	9.91783298	5.27885294
H	29.18170062	9.07362104	5.38525040
C	36.63990320	15.55197569	4.36964959
H	35.93279053	14.72083214	4.46024606
C	36.13878458	16.87604126	4.37112388
C	38.41668476	17.72929261	4.13840526
H	39.12646867	18.56412650	4.04643252
C	38.91635490	16.41070503	4.13738920
C	38.01470287	15.33456709	4.25314104
H	38.41884892	14.31152459	4.24917472
C	37.04767132	17.95902709	4.25352629
H	36.66055232	18.99083497	4.25344173
C	40.37227903	16.16338941	4.01515516
O	43.74513544	18.13845229	3.60529567
O	45.47863261	16.76709126	3.64372713
H	45.68298800	18.82794573	3.62274732
C	44.98056455	17.95156871	3.62443342
N	46.94883686	15.12707000	5.02263688
H	46.31772759	14.38912746	4.56030683
H	46.57617963	15.98436840	4.48960267
C	48.37398555	14.88265155	4.74034005
H	48.98828437	15.71705407	5.13032350
H	48.70098561	13.93993552	5.21998724
H	48.51730744	14.80421451	3.64676791
C	46.58021920	15.25119926	6.44984385
H	45.48935771	15.43277812	6.51063363
H	46.83640911	14.31816400	6.98764004
H	47.12755972	16.09745253	6.90781400

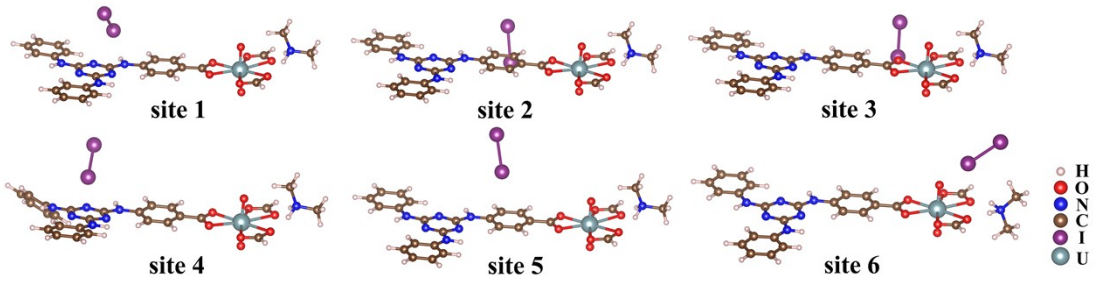

Figure S1. Optimized structures of I_2 molecule adsorbed at different sites on cluster model at PBE-D3 level of theory.

Table S2. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 1 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.09268636	15.68690852	3.67718042
O	43.27521232	15.74053196	5.46620635
O	43.06421179	15.60859877	1.89571347
O	42.92197093	13.17084269	3.75593033
O	45.00355044	13.91606230	3.78207379
C	44.15097519	12.95566618	3.82587993
H	44.53356698	11.90453260	3.92727365
O	41.17794592	17.12236972	3.74456090
O	40.82273578	14.95094640	3.85042047
N	32.48864294	17.13013239	4.49543610
N	33.71857605	15.07150824	4.52815349
N	31.33943165	15.05161609	4.84010268
N	30.15834810	17.00740290	4.83179202
H	29.41931423	16.32286165	5.00443297
N	34.75846947	17.16772805	4.23095560
H	34.53365602	18.16636540	4.18797264
N	32.63771041	13.08279843	4.83507214
H	33.60772474	12.77647655	4.73405721
H	28.39578469	22.03732974	4.79079258
C	28.77382768	21.00440974	4.79275622
C	28.39026951	18.61737719	5.06138007
H	27.70517972	17.78011958	5.27226588
C	30.62554383	19.42926610	4.53179164
H	31.68110313	19.21907780	4.33004014
C	27.90761287	19.93021871	5.05503848
H	26.84185741	20.11370443	5.25973119
C	30.12697608	20.73891194	4.53323696
H	30.82263823	21.56744692	4.32787368
C	29.75583935	18.34965367	4.80258060
C	31.38494393	16.40395109	4.71182625
C	32.52901453	14.44687482	4.73396258
C	33.63320283	16.40233739	4.42263059
C	31.69449939	12.06798848	5.04549961
C	31.31053332	9.66614637	5.29810728
H	31.71381876	8.64257380	5.32929204
C	30.30963328	12.29480729	5.21246782
H	29.93690963	13.32405420	5.17583581
C	32.18232822	10.73978702	5.09094843
H	33.26108323	10.55547243	4.96086933

C	29.44969088	11.20717300	5.41923414
H	28.37318479	11.39942361	5.54752882
C	29.93418756	9.89100428	5.46444442
H	29.24738704	9.04741898	5.62725130
C	36.62007045	15.52360863	4.15061651
H	35.91513504	14.69036573	4.23753259
C	36.11465084	16.84610531	4.14032490
C	38.39241380	17.70538358	3.93264130
H	39.10051931	18.54247043	3.84856097
C	38.89656045	16.38832141	3.94288101
C	37.99678345	15.30987294	4.05195394
H	38.40396447	14.28805701	4.05703421
C	37.02161886	17.93186175	4.03001198
H	36.62928015	18.96116032	4.02949860
C	40.35402872	16.14446660	3.84148567
O	43.73853047	18.12175978	3.52583344
O	45.47055963	16.75335773	3.65130673
H	45.67373186	18.81374642	3.60751832
C	44.97239807	17.93655156	3.59522447
N	46.88024384	15.12805283	5.10888267
H	46.26796358	14.38413942	4.63006272
H	46.52891078	15.97838667	4.55066679
C	48.31564411	14.88221899	4.88748145
H	48.91313256	15.71981777	5.29637069
H	48.62287463	13.94327610	5.38719829
H	48.50399511	14.79593186	3.80134365
C	46.45409589	15.26841100	6.51848404
H	45.36087395	15.44508613	6.53299866
H	46.69254410	14.34348335	7.07802650
H	46.97885869	16.12297748	6.98734677
I	33.62425104	19.46966824	7.34689388
I	34.24001552	21.00329636	5.19822305

Table S3. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 2 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.10066403	15.66784004	3.78000255
O	43.35109249	15.67385847	5.56156344
O	43.00338735	15.63721913	1.99933395
O	42.93458011	13.15032719	3.78992492
O	45.01585239	13.89624350	3.77071734
C	44.16523989	12.93428378	3.81469601
H	44.55084819	11.88109139	3.87452099

O	41.19199292	17.09789940	3.96013866
O	40.83748182	14.92457348	4.01935726
N	32.50959118	17.12628804	4.74041074
N	33.71803552	15.05427728	4.69298395
N	31.32838092	15.04440412	4.91289013
N	30.16450395	17.01005376	4.95300420
H	29.41193554	16.32428162	5.04275563
N	34.78455074	17.15184469	4.53502422
H	34.56613953	18.15069695	4.52847465
N	32.60848130	13.06456543	4.85875419
H	33.57870701	12.75312530	4.77712981
H	28.40571241	22.04159378	4.93538178
C	28.78442753	21.00893098	4.93778194
C	28.38135342	18.61381706	5.05815056
H	27.67945902	17.76910654	5.15077517
C	30.66062405	19.44376808	4.82355021
H	31.73283271	19.23921720	4.73378115
C	27.89785953	19.92609734	5.05574357
H	26.81523894	20.10203943	5.14701411
C	30.15930939	20.75291702	4.82272414
H	30.86697307	21.59113607	4.72900300
C	29.76820260	18.35447488	4.94221466
C	31.39066345	16.40103693	4.86360384
C	32.51579484	14.43271102	4.82329299
C	33.64761832	16.38919905	4.65958926
C	31.64900454	12.05032383	4.98142283
C	31.23499630	9.64290672	5.09360902
H	31.62786696	8.61485070	5.08595233
C	30.26103586	12.28306310	5.10942169
H	29.89876490	13.31666137	5.11348926
C	32.12325616	10.71651485	4.97508106
H	33.20445559	10.52771258	4.87517473
C	29.38449048	11.19539383	5.22726895
H	28.30572899	11.39218641	5.32630700
C	29.85546352	9.87357487	5.22100735
H	29.15571379	9.03007206	5.31429179
C	36.63767673	15.50056797	4.40148877
H	35.92999631	14.66857537	4.47923242
C	36.13808522	16.82516963	4.42241252
C	38.41573444	17.68009959	4.20355870
H	39.12295222	18.51848660	4.12395938
C	38.91456945	16.36157469	4.18084317
C	38.01236222	15.28399931	4.28077325

H	38.41569078	14.26082764	4.26031105
C	37.04726198	17.90865267	4.32204643
H	36.66547811	18.94232557	4.33827235
C	40.36957984	16.11788028	4.04932408
O	43.73913721	18.10632555	3.66172190
O	45.47573887	16.73822810	3.69112683
H	45.67547907	18.79941852	3.69046058
C	44.97483308	17.92164768	3.68199472
N	46.94262029	15.08000961	5.05096167
H	46.31337853	14.34854452	4.57508607
H	46.57166609	15.94474597	4.52892676
C	48.36912879	14.84050112	4.77230001
H	48.98139258	15.66712514	5.18161367
H	48.69319945	13.88874832	5.23581307
H	48.51877196	14.78290480	3.67826435
C	46.56706148	15.18261846	6.47809354
H	45.47560450	15.36148749	6.53643996
H	46.82188345	14.24207420	7.00334584
H	47.11109962	16.02266617	6.95116301
I	38.15989002	21.85989609	4.79674907
I	38.21743827	21.26184487	2.15255635

Table S4. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 3 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.11602729	15.66606439	3.73670966
O	43.34802210	15.65007718	5.52105863
O	43.03769972	15.65912226	1.95462026
O	42.94205253	13.14887113	3.70961192
O	45.02454389	13.89235326	3.71924257
C	44.17220786	12.93089577	3.74003380
H	44.55615822	11.87636297	3.78419265
O	41.21294043	17.09991092	3.90883685
O	40.84627036	14.92912423	3.95017671
N	32.52706446	17.15251833	4.68368766
N	33.73657240	15.08074041	4.66804341
N	31.34862912	15.07361019	4.90478958
N	30.18323802	17.03848535	4.91338586
H	29.43201053	16.35376366	5.02081908
N	34.80092435	17.17574108	4.46464520
H	34.58100663	18.17400923	4.44448827
N	32.62987272	13.09397748	4.88219694
H	33.59985452	12.78155721	4.80146437

H	28.41653901	22.06601660	4.80322105
C	28.79685298	21.03416570	4.82443444
C	28.39814951	18.64140228	4.99492911
H	27.69805972	17.79769006	5.10799666
C	30.67492968	19.46982029	4.73249555
H	31.74699508	19.26500031	4.64173287
C	27.91256731	19.95263773	4.96849483
H	26.83014252	20.12879582	5.06154298
C	30.17155582	20.77795140	4.70784971
H	30.87731212	21.61528643	4.59406954
C	29.78480531	18.38189317	4.87737089
C	31.40928455	16.42899754	4.82797396
C	32.53574490	14.46091357	4.81952580
C	33.66481217	16.41454184	4.60973645
C	31.67233372	12.08192958	5.03538543
C	31.26172544	9.67741751	5.20591006
H	31.65554989	8.64978422	5.21876547
C	30.28520121	12.31642646	5.16879176
H	29.92187179	13.34951426	5.15203941
C	32.14793153	10.74877148	5.05579418
H	33.22851212	10.55863952	4.95180599
C	29.41071135	11.23101590	5.31846282
H	28.33256384	11.42910700	5.42144569
C	29.88301028	9.90982117	5.33884345
H	29.18488034	9.06809813	5.45699535
C	36.65042111	15.52178989	4.33444582
H	35.94098655	14.69199078	4.41890315
C	36.15370458	16.84748890	4.35006765
C	38.43395166	17.69589959	4.12232471
H	39.14176172	18.53242041	4.03766768
C	38.92948709	16.37559179	4.10727132
C	38.02423218	15.30121992	4.21271432
H	38.42492848	14.27692294	4.19724114
C	37.06592351	17.92830319	4.24112715
H	36.68410327	18.96198668	4.25147740
C	40.38357654	16.12426953	3.98328289
O	43.76087792	18.09818381	3.66303828
O	45.50101424	16.73649727	3.68871116
H	45.69263420	18.79936073	3.72639999
C	44.99740018	17.91824994	3.69408142
N	46.94186091	15.04836838	5.04069716
H	46.31440442	14.32780081	4.54650615
H	46.58158925	15.92346519	4.52906725

C	48.37010687	14.80672087	4.77236439
H	48.98179691	15.62329465	5.20215098
H	48.68509161	13.84556881	5.22251705
H	48.53057914	14.76743244	3.67906225
C	46.55216183	15.12683733	6.46559057
H	45.46108270	15.31036454	6.51625734
H	46.79630120	14.17488867	6.97514983
H	47.09613243	15.95439815	6.96020276
I	41.53746628	20.45162424	5.36183741
I	41.31551028	20.58345973	2.66667196

Table S5. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 4 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.06907995	15.81463725	3.80118934
O	43.28872487	15.45905425	5.55041257
O	42.99743340	16.14463700	2.05037519
O	42.89472093	13.34800975	3.30597372
O	44.97713861	14.07441416	3.46063748
C	44.12486039	13.12648737	3.29972662
H	44.50797375	12.08161308	3.14907133
O	41.15537401	17.18961283	4.24887352
O	40.79597422	15.05336102	3.84523489
N	32.45608182	17.02313266	5.02663478
N	33.71015137	15.01781554	4.66441582
N	31.33144668	14.91153184	4.96503959
N	30.11075853	16.83765806	5.16386688
H	29.37453051	16.15020449	5.33867345
N	34.73838631	17.13148064	4.74338244
H	34.53091151	18.11660051	4.94796322
N	32.66982914	12.98793516	4.72561285
H	33.64622126	12.71272933	4.59657045
H	28.39894069	21.83639490	4.48492505
C	28.76026425	20.80639805	4.61967350
C	28.56234491	18.62450816	5.67561836
H	28.05274170	17.94347891	6.37468841
C	30.36513701	19.04894129	4.09043840
H	31.24989692	18.70204644	3.54162335
C	28.09411763	19.93101690	5.49206999
H	27.20597786	20.27032024	6.04595195
C	29.89177686	20.35627129	3.92229016
H	30.41965786	21.03234598	3.23316066
C	29.70380910	18.17570110	4.97952067

C	31.34220569	16.26016899	5.04337488
C	32.53645542	14.34698767	4.79674120
C	33.62663327	16.34176703	4.80729151
C	31.74346381	11.93512780	4.78924674
C	31.41097328	9.51496356	4.71960507
H	31.83622693	8.50433818	4.62601598
C	30.35214326	12.11212232	4.95700719
H	29.95460727	13.12854269	5.04796611
C	32.26174905	10.62379427	4.67176232
H	33.34653316	10.48007171	4.54083011
C	29.51322719	10.98986260	5.00178130
H	28.43067478	11.14169128	5.13204939
C	30.02730854	9.68956048	4.88502442
H	29.35691903	8.81842807	4.92291696
C	36.59672656	15.54646074	4.26608218
H	35.89231306	14.71824362	4.13926107
C	36.09793026	16.83000348	4.58802525
C	38.37434599	17.71002505	4.60316209
H	39.08450772	18.53970869	4.73094704
C	38.87388143	16.43097420	4.28369091
C	37.97380699	15.36063568	4.11941886
H	38.38020277	14.36998974	3.86789121
C	37.00339958	17.90763583	4.75527207
H	36.61358954	18.90536994	5.01305263
C	40.33290126	16.21608844	4.11991696
O	43.71007350	18.22101933	4.18337860
O	45.44489540	16.86750645	3.97073490
H	45.64567231	18.88704808	4.38448069
C	44.94543204	18.03131314	4.18873573
N	46.88231500	14.95866298	4.99583446
H	46.26200755	14.34371556	4.36887355
H	46.52151493	15.91341383	4.65630089
C	48.31347432	14.77670821	4.69675914
H	48.91883009	15.49787804	5.27907201
H	48.62938383	13.74817033	4.95743574
H	48.48133773	14.94745541	3.61727952
C	46.48307657	14.76600837	6.40726670
H	45.39099205	14.93363034	6.48385053
H	46.72887555	13.73630685	6.73076733
H	47.01989740	15.48804450	7.05209638
I	33.28789437	21.21964659	8.44164466
I	32.72030545	19.13966722	6.66743731

Table S6. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 5 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	43.12479792	15.65473203	3.66728961
O	43.33122409	15.67123287	5.45251062
O	43.06084865	15.61309034	1.88608690
O	42.94032707	13.14417553	3.69037620
O	45.02528387	13.87848152	3.71027615
C	44.16944095	12.92072695	3.73981173
H	44.54732360	11.86568411	3.80941369
O	41.20732049	17.09729971	3.80132103
O	40.84129591	14.92331839	3.86336872
N	32.53025810	17.11918977	4.64511058
N	33.74092010	15.05218602	4.53921014
N	31.36149154	15.03346629	4.84889718
N	30.19533356	16.99597888	4.94670894
H	29.44648183	16.30883390	5.05638763
N	34.79436967	17.15584355	4.35187366
H	34.57174957	18.15369797	4.38484932
N	32.64301926	13.05761684	4.73674758
H	33.61043114	12.74806910	4.62167906
H	28.42750987	22.02267838	5.06887694
C	28.80811880	20.99112792	5.04083232
C	28.41226905	18.59339139	5.11825729
H	27.71429366	17.74510074	5.20746225
C	30.68481388	19.43388714	4.85591610
H	31.75572815	19.23562299	4.74186347
C	27.92604055	19.90419812	5.15349710
H	26.84526202	20.07564802	5.27065413
C	30.18098575	20.74153713	4.89322722
H	30.88496327	21.58336004	4.80554425
C	29.79682917	18.34097246	4.96910726
C	31.41580077	16.39023576	4.80680946
C	32.54477682	14.42385109	4.71204151
C	33.66086298	16.38418948	4.51858627
C	31.69099983	12.03934890	4.89172554
C	31.29026211	9.63066363	5.01090248
H	31.68596261	8.60403898	4.98579315
C	30.30837071	12.26750822	5.07144232
H	29.94224342	13.29944076	5.09317859
C	32.16983975	10.70780314	4.86338403
H	33.24733849	10.52318364	4.72370075

C	29.44042197	11.17635372	5.21778089
H	28.36548260	11.36888956	5.35754771
C	29.91567618	9.85643655	5.18961545
H	29.22273717	9.01022456	5.30599582
C	36.64361424	15.50968024	4.21503052
H	35.93596216	14.67760392	4.28986659
C	36.13907321	16.83187986	4.24144232
C	38.43639742	17.68645145	4.02917132
H	39.14673830	18.52183132	3.94690276
C	38.92768879	16.36963325	4.00579361
C	38.01847212	15.29580085	4.09709127
H	38.42197787	14.27258028	4.07631485
C	37.05783258	17.92274857	4.15151823
H	36.67016380	18.95248862	4.09682311
C	40.38619054	16.11913831	3.88508097
O	43.76495360	18.08511438	3.54201401
O	45.49743890	16.71527276	3.62777663
H	45.70121978	18.77655325	3.60672627
C	45.00019785	17.89970978	3.59287096
N	46.92740991	15.06027876	5.03861545
H	46.30859843	14.32887982	4.55182590
H	46.57268958	15.92308336	4.50463582
C	48.35953336	14.81563984	4.79229249
H	48.96435755	15.64210096	5.21259192
H	48.66996721	13.86467149	5.26642164
H	48.53321561	14.75390734	3.70207343
C	46.52170397	15.16968890	6.45744278
H	45.42975373	15.35044789	6.49294115
H	46.76436848	14.23098751	6.99148085
H	47.05707556	16.01096976	6.93789884
I	37.10480128	18.94787295	9.78700098
I	37.28873086	18.35843079	7.08859054

Table S7. The Cartesian coordinates of optimized structures of I_2 molecule adsorbed at site 6 on cluster model at PBE-D3 level of theory.

atom	*x*	*y*	*z*
U	42.94307626	15.82253125	4.57113987
O	43.06100137	16.03284471	6.38204208
O	42.97540300	15.59413780	2.80143522
O	42.79150911	13.34804141	4.92725469
O	44.85668306	14.11198177	4.79957881
C	44.02631065	13.15009924	4.97944356
H	44.42577021	12.12279290	5.18728145

O	41.02724645	17.23020142	4.45795060
O	40.68864326	15.07043917	4.70050353
N	32.30847255	17.16625897	4.57791468
N	33.54548788	15.11534272	4.71045136
N	31.14626576	15.07163594	4.72294674
N	29.95544224	17.01756372	4.60382804
H	29.20758702	16.32257205	4.65435292
N	34.59190033	17.22422868	4.55849070
H	34.35822940	18.21682534	4.48401876
N	32.45355311	13.11306695	4.84491576
H	33.43130415	12.81520319	4.86112855
H	28.12924227	22.01606657	4.30509751
C	28.52193383	20.99047664	4.36606331
C	28.14624478	18.59279531	4.51772891
H	27.45184540	17.73885507	4.57571531
C	30.42443937	19.45554244	4.44862155
H	31.50336060	19.26750303	4.45325681
C	27.64492932	19.89603155	4.44004713
H	26.55597482	20.05568327	4.43762729
C	29.90531119	20.75544807	4.37134396
H	30.60541209	21.60324235	4.31407080
C	29.54161696	18.35475315	4.52309306
C	31.19242781	16.42666573	4.63408837
C	32.34484942	14.47685638	4.75685860
C	33.45780973	16.44567598	4.62030317
C	31.50113993	12.08621138	4.91060183
C	31.11419638	9.67687026	5.06417797
H	31.52106008	8.65638170	5.12983348
C	30.10422829	12.29825533	4.89573625
H	29.72753660	13.32454094	4.82981190
C	31.99374682	10.76194587	4.99583807
H	33.08222717	10.58955625	5.00815567
C	29.23655408	11.19930695	4.96491983
H	28.15049580	11.37963565	4.95222030
C	29.72558989	9.88679473	5.04920176
H	29.03264176	9.03430016	5.10286049
C	36.46750184	15.60224908	4.68694327
H	35.76448594	14.76696146	4.77124434
C	35.95241666	16.91639895	4.57021398
C	38.23127101	17.79187081	4.46157370
H	38.93536711	18.63191147	4.37393844
C	38.74427167	16.48286044	4.57799390
C	37.84889178	15.40030066	4.69087904

H	38.26267200	14.38523888	4.78208894
C	36.85552997	18.00564033	4.45895653
H	36.45783243	19.02926120	4.36847560
C	40.20388008	16.25272657	4.57915402
O	43.55358862	18.23715404	4.29503973
O	45.28641888	16.88140559	4.44206954
H	45.48944228	18.93920869	4.30923210
C	44.79161498	18.06187484	4.34557489
N	47.23879048	15.18888135	4.82883890
H	46.43291260	14.51329907	5.02223534
H	46.67160509	16.09631559	4.80461521
C	47.72180391	14.92589334	3.45616255
H	48.45892926	15.69672377	3.16115836
H	48.19668112	13.92748397	3.40764327
H	46.85560128	14.95845410	2.77048076
C	48.27050034	15.17998261	5.88439425
H	47.79896498	15.39901648	6.86071208
H	48.75628333	14.18649323	5.92753062
H	49.03530270	15.94977657	5.66709882
I	47.14917281	15.95652715	9.83977489
I	44.97868279	16.00252936	8.10791749

Table S8. The lattice parameters of the periodic UOF at spin multiplicity of 1 and 3 with U_{eff} values ranging from 0–6.

	Lattice parameters							
	Spin multiplicity of 1				Spin multiplicity of 3			
U_{eff} (eV)	a(Å)	b(Å)	c(Å)	V(Å^3)	a(Å)	b(Å)	c(Å)	V(Å^3)
0	31.918	18.606	13.154	7787.36	31.919	18.610	13.224	7830.60
1	31.919	18.607	13.148	7783.96	31.919	18.610	13.224	7830.58
2	31.919	18.606	13.143	7780.72	31.919	18.610	13.224	7830.59
3	31.919	18.605	13.134	7775.20	31.919	18.610	13.224	7830.56
4	31.919	18.606	13.160	7791.01	31.919	18.614	13.217	7828.04
5	31.919	18.606	13.161	7791.82	31.919	18.614	13.216	7827.46
6	31.919	18.608	13.207	7819.99	31.916	18.609	13.204	7817.55

Table S9. The energies of the periodic UOF system at spin multiplicity of 1 and 3 with U_{eff} values ranging from 0–6.

	Energy (a.u.)	
U_{eff} (eV)	spin multiplicity of 1	spin multiplicity of 3
0	-3285.126	-3285.044
1	-3284.927	-3284.839
2	-3284.735	-3284.637
3	-3284.552	-3284.446
4	-3284.374	-3284.269
5	-3284.202	-3284.098
6	-3284.027	-3283.934

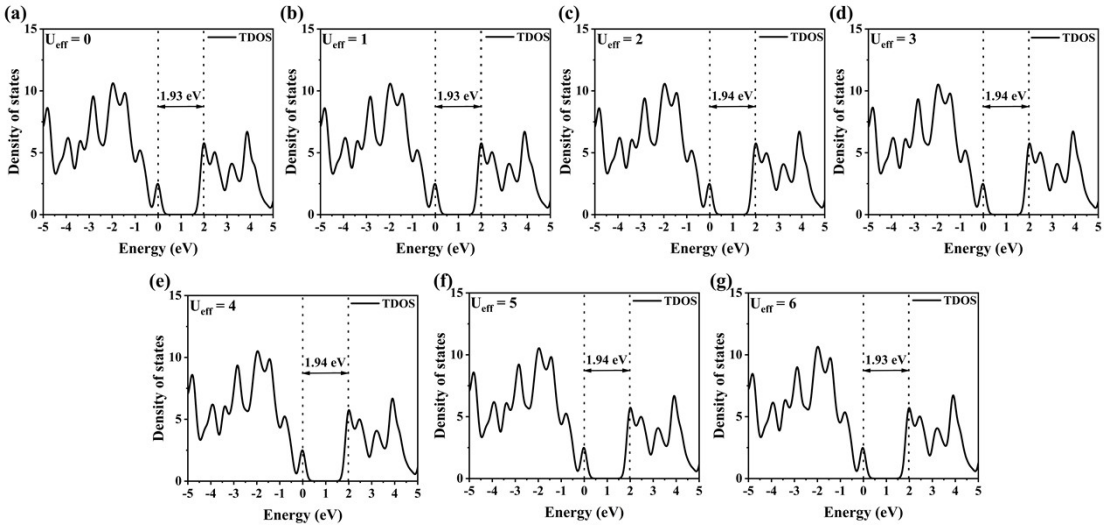

Figure S2. (a-g) Density of states (DOS) of the periodic UOF system with U_{eff} values ranging from 0–6 eV. The Fermi levels are set to zero.

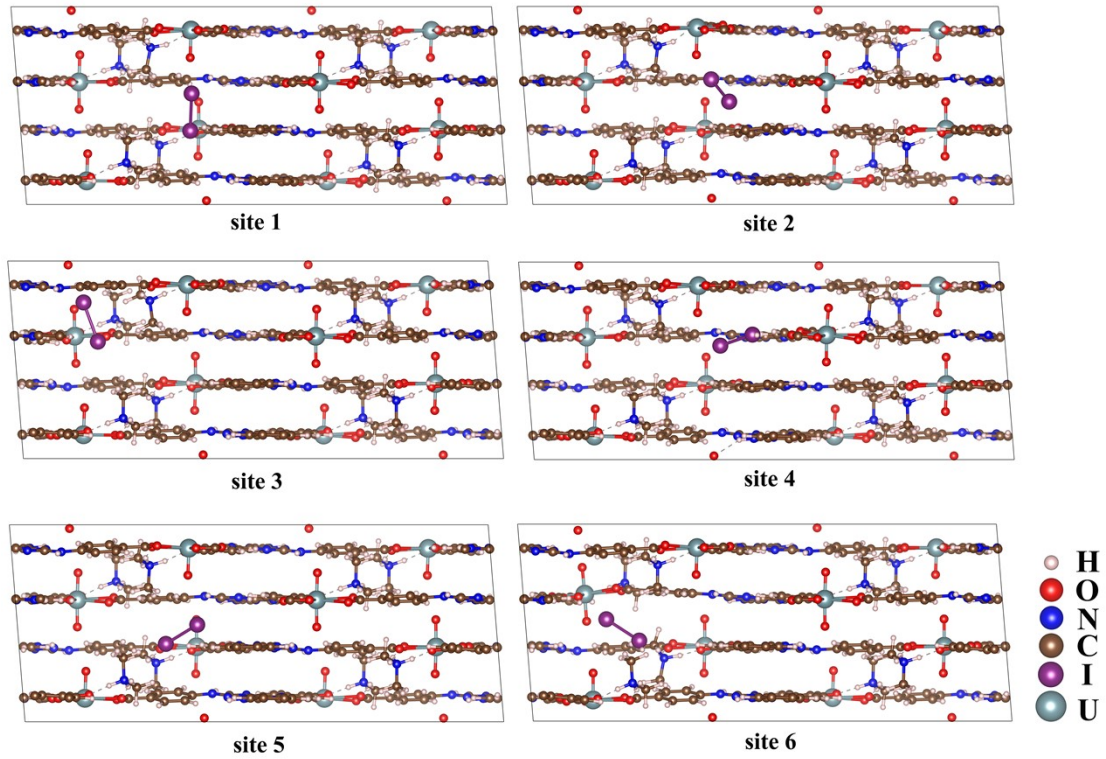

Figure S3. Optimized structures of I_2 molecule adsorbed at different sites in the periodic UOF model.