Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

-Supporting Information-

Energy-based Descriptors for Photo-Catalytically Active Metal-Organic Frameworks Discovery

Maria Fumanal*[1,2], Gloria Capano[1], Senja Barthel,[1,3] Berend Smit[1], Ivano Tavernelli*[2]

[1]Laboratory of Molecular Simulation, Institut des Sciences et Ingénierie Chimiques, Valais, Ecole Polytechnique Fédérale de Lausanne (EPFL), Rue de l'Industrie 17, CH-1951, Sion, Switzerland

[2]IBM Research Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

[3]Department of Mathematics, Vrije Universiteit Amsterdam, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands

*maria.fumanal@epfl.ch, *ITA@zurich.ibm.com

Section S1. Electronic Chemical Potential

We modified the available MacroDensity package[1,2] to be applied for output files of CP2K, which are given in standard cube format. In a first step, the potential, lattice vectors and atomic coordinates are read from the output cube file. Then, each point of the grid spaced a certain threshold (we used 0.2/lattice-vector in reciprocal space) is potentially considered for the calculation of the potential average within a cube size of 40x40x40 in grid mesh points (about 2.5 Å^3). Grid points with a distance below 2 Å to an atom are automatically discarded. The vacuum potential is given by the potential average of the cube-grid with the smallest variance. The modified SphericalAverage.py python code reads as follows:

```
input_file = 'TEST.cube'
cube_size = [40,40,40]

pot,NGX,NGY,NGZ,Lattice,num_atoms,coord,atom_type=read_cube_density(input_file)
vector_a,vector_b,vector_c,av,bv,cv = md.matrix_2_abc(Lattice)
resolution_x = vector_a/NGX
resolution_y = vector_b/NGY
resolution_z = vector_c/NGZ
c1=0.2/vector_a
c2=0.2/vector_b
c3=0.2/vector_c
grid_pot = md.density_grid_cube(pot,NGX,NGY,NGZ)

cube = cube_size

travelled = [0,0,0]

params = cell_to_cellpar(Lattice,radians=False)
thr=2.0
cube_var_l=1000
cube_potential_l=0
d_l=0
f_l=0
g_l=0
logical=0
for d in np.arange(0.0,1.0,c1):
   for f in np.arange(0.0,1.0,c2):
      for g in np.arange(0.0,1.0,c3):
         cube_origin = [d,f,g]
         logical = test_point(cube_origin,coord,params,num_atoms,thr)
         if logical == 1:
            cube_potential,cube_var =md.cube_potential(cube_origin,travelled,cube,grid_pot,NGX,NGY,NGZ)
            if cube_var < cube_var_l:
               cube_var_l=cube_var
               cube_potential_l=cube_potential
               d_l=d
               f_l=f
               g_l=g

print(" %4.1f %5.2f %5.2f %5.2f %10.4f %10.6f "%(thr,d_l,f_l,g_l,cube_potential_l,cube_var_l))
```

[1] Butler, K. T.; Hendon, C. H.; Walsh A. Electronic Chemical Potentials of Porous Metal−Organic Frameworks *J. Am. Chem. Soc.* **2014**, *136*, 2703−2706

[2] https://github.com/WMD-group/MacroDensity

Figure S1 shows some examples of structures for which the center of the pore is not appropriate given the structural topology of the ligands, and thus displaced positions inside the pore provide the most accurate potential plateau for the electrostatic potential.

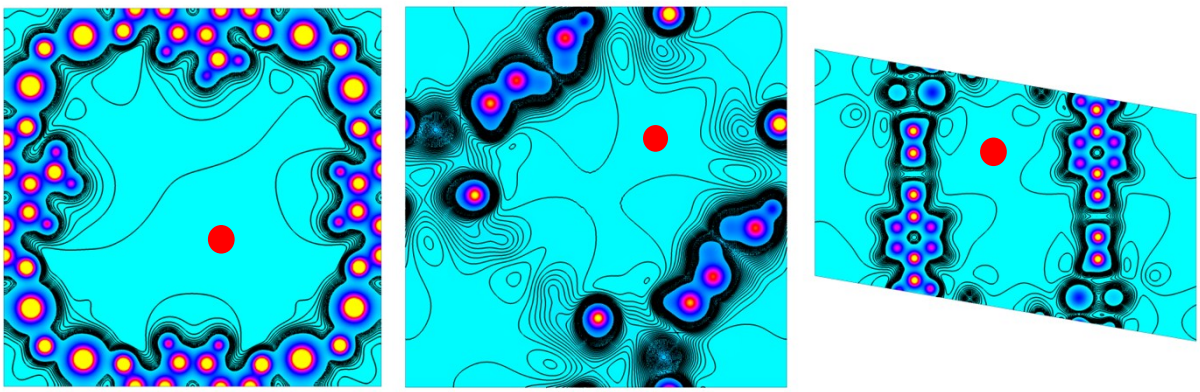

Figure S1. Slice through the electrostatic potential of three different DS2 MOFs. The red points represent the point with the lowest average plateau considering a 40x40x40 grid-points cube.

Section S2. Band gap k-points analysis

Γ-point and extended 2x2x2 k-point sampling was used to evaluate the electronic band gap of **DS1** and **DS2** structures. The results obtained for **DS1** are shown in **Figure S1a** and the raw data is collected in Table S3. For those cases with a deviation above 0.25 eV (28 **DS1** structures), the k-point sampling was optimized based on the ratio between the a,b,c unit cell parameters (kx) and the band gap was compared with the standardized 2x2x2 sampling (**Figure S1b**). The results show that the optimized k-point sampling implies a significant correction of the band gap (>0.3 eV) in only 3 cases, while it remains negligible for the rest (Table S4).

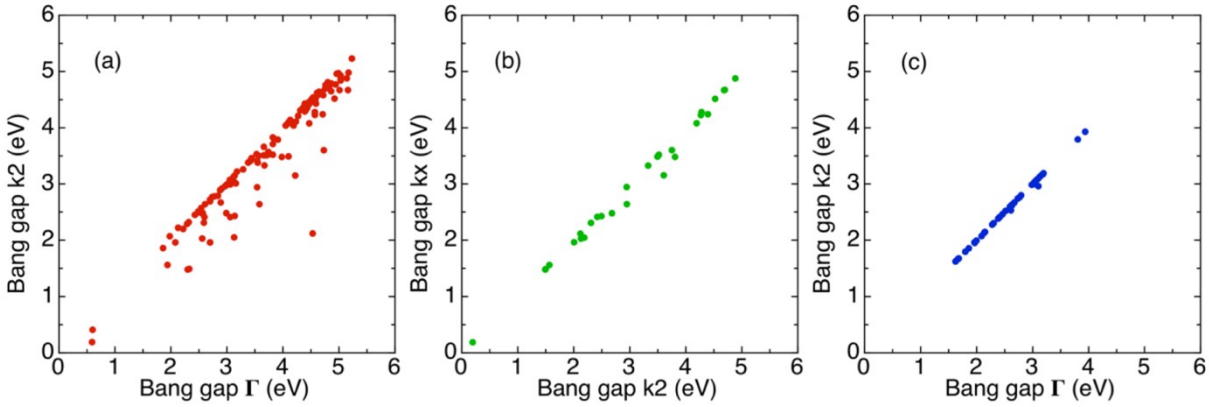

Figure S1. PBE electronic band gap of (a) all **DS1** computed at Γ and using a 2x2x2 k-point sampling (k2), (b) 28 selected MOFs of **DS1** computed using k2 sampling and an optimized k-point sampling (see Table S4), (c) all **DS2** computed at Γ and with k2.

The choice of 0.25 eV as threshold to consider that k-point sampling is necessary is made considering that this criteria provides a very good correlation between the Γ-point and extended k-point sampling band gap results as shown in Figure S2. Moreover, a tighter criteria will extremely reduce the number of candidates for LR-TDDFT calculations, for which Γ-point sampling is required.

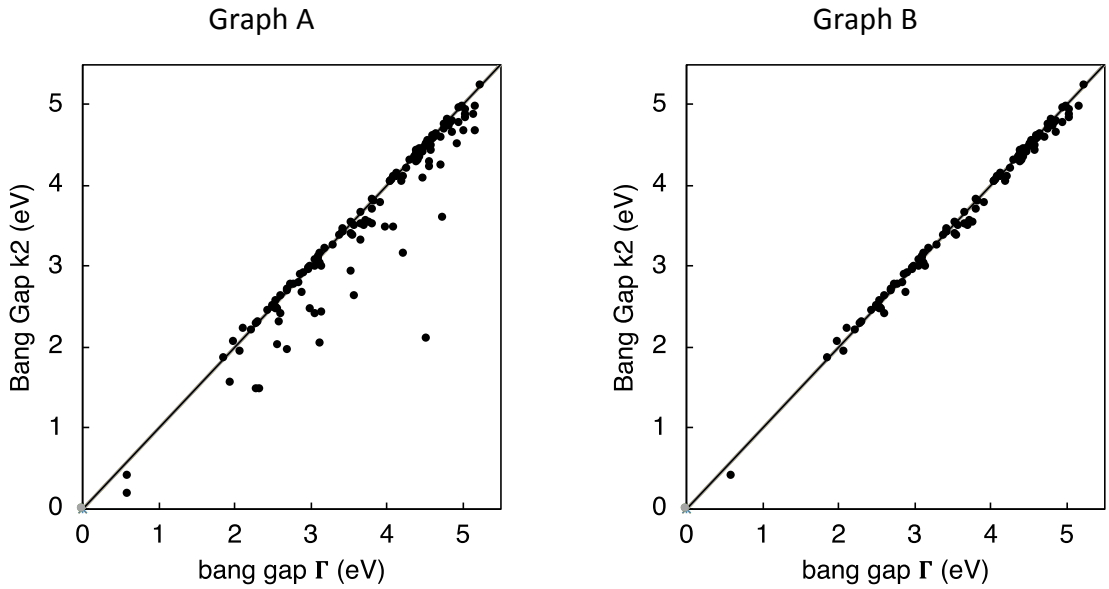

Figure S2. PBE electronic band gap of all DS1 computed at Γ and using a 2x2x2 k-point sampling (Graph A) and when excluding those DS1 systems with ΔE_k > 0.25 eV (Graph B).

We performed an analysis of the dependence of the difference between the band gap at Γ-point and when including 2x2x2 k-point sampling (ΔE_k), with the unit cell volume (**Figure S3a**) and with the maximum ratio between a,b,c unit cell parameters (**Figure S3b**) On the one hand, the results show that there is no direct correlation between the unit cell volume and the magnitude of ΔE_k. Contrarily, ΔE_k of ~1 eV can be found for unit cell volumes from 500 Å^3 to 1000 Å^3, as well as negligible differences are obtain in the full range of explored volumes (**Figure S3a**). On the other hand, the data mapped in **Figure S3b** points to a sizeable correlation between the maximum possible cell parameters ratio and the need of including extended k-point sampling. In particular, ΔE_k > 1 eV only appear for maximum cell ratios above 2.2, while the maximum ΔE_k value explored of 2.5 eV is obtained for the maximum cell parameters ratio considered of 4. However, other structures with maximum cell ratios of 4 provide converged band gaps at Γ-point. In order to determine if there is a simultaneous correlation between the cell parameters ratio and the volume with ΔE_k we present a two-variable plot in **Figure S4**. It can be seen that no direct correlation can be made and that systems with similar descriptors show very different ΔE_k values. The lack of a correlation between ΔE_k with the structural unit cell characteristics prevents the direct association of a particular shape with the need of extended k-point sampling.

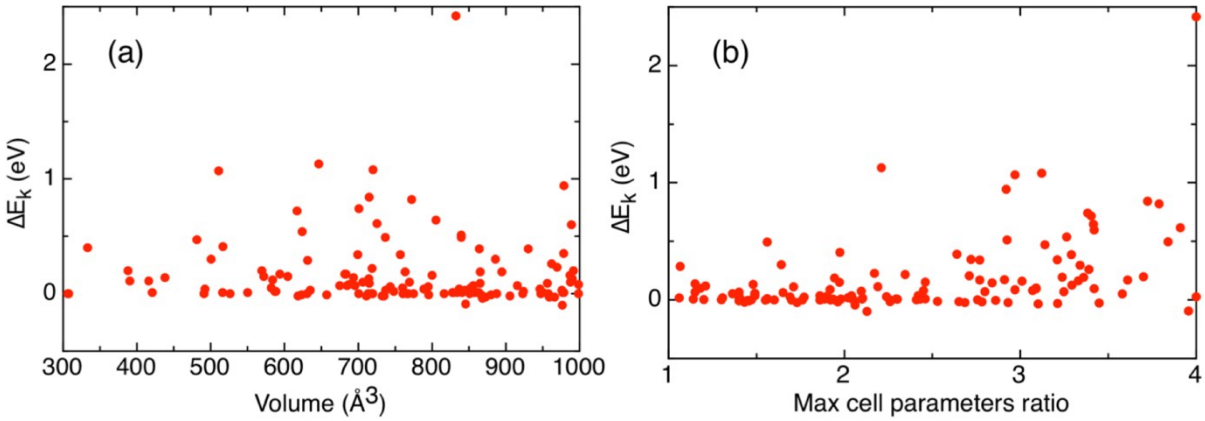

Figure S3. Dependence of the absolute difference between the computed PBE band gap of **DS1** at Γ and when using a 2x2x2 k-point sampling (ΔE_k) (a) with the unit cell volume (in $Å^3$) and (b) with the maximum ratio between a/b/c cell parameters.

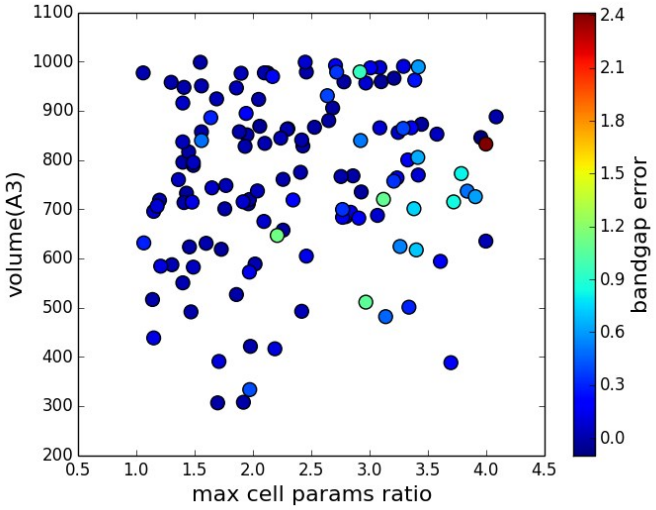

Figure S4. Dependence of the absolute difference between the computed PBE band gap of **DS1** at Γ and when using a 2x2x2 k-point sampling (ΔEk band gap error in color code) with the maximum ratio between a/b/c cell parameters (x) and with the unit cell volume (in Å3) (y).

Figure S5 shows the direct correlation between the electronic band gap computed at PBE and PBE0 levels. The linear regression indicates a systematic shift of 2.15 eV. At PBE0 level the exciton binding energies corresponding to the energy difference between the electronic band gap and the lowest excited S_1 energy are -1.35 eV (Figure 3b of main text). Altogether the direct correlation between the PBE band gap and the PBE0 S_1 energies provides a shift of +0.85 eV as shown in Figure 3c of the main text.

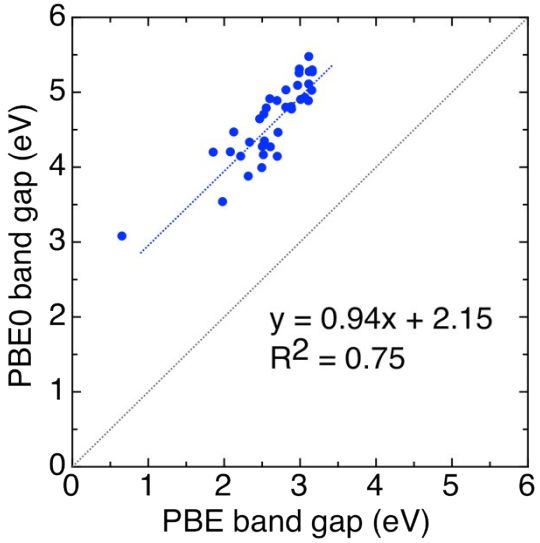

Figure S5. Correlation between the computed PBE and PBE0 band gaps of DS1 structures.

Table S1. **DS1** MOF structures. Cell parameters a/b/c and volume are given in Å. Angles in °.

CSD code	Chemical composition	a	b	c	alpha	beta	gamma	volume
ASALEL	'(C8 H7 N1 O3 Zn1)n'	5.3597(5)	9.9042(10)	15.6760(16)	90	90	90	832.14
BENKOW	'(C2 H4 N3 O4 P1 Zn1)n'	8.5467(13)	8.4344(12)	8.9674(13)	90	90	90	646.43
BENQUH	'(C3 H6 Na1 O6 P1 Zn1)n'	5.2220(10)	15.519(3)	8.883(2)	90	90.63(3)	90	719.84
BUKJIA	'(C8 H4 N8 Zn1)n'	7.1189(2)	9.6994(4)	7.3988(3)	90	90	90	510.88
BUWLEL01	'(C10 H18 N4 O6 Zn1)n,2n(C1 H4 O1)'	14.109(16)	14.455(17)	4.799(6)	90	90	90	978.74
CAKLOR	'(C12 H16 O8 Zn2)n'	16.1050(12)	4.7876(4)	9.2686(7)	90	90.024(4)	90	714.65
CAVQOH	'(C4 H12 N2 O12 P4 Zn3)n'	10.6881(3)	13.3129(3)	5.4266(2)	90	90	90	772.15
CIMFIP	'(C4 H3 N3 O4 Zn1)n'	14.268(3)	4.5707(11)	10.746(3)	90	90	90	700.80
CIMZII	'(C4 H6 O6 Zn1)n'	7.777(5)	8.882(5)	8.933(5)	90	90	90	617.05
CUJBAK	'(C8 H12 O14 Zn2)n,3n(H2 O1)'	11.2499(10)	7.9548(7)	8.9966(7)	90	90	90	805.11
CUMBAO	'(C4 H9 N1 O6 Zn1)n'	5.2512(1)	9.7224(3)	14.2052(4)	90	90	90	725.24
DASLOZ	'(C8 H10 N2 O6 Zn1)n'	9.05934(17)	7.44099(10)	14.66969(22)	90	90	90	988.89
DEHYEV	'(C2 H2 O5 P1 Zn1 1-)n,n(H3 O1 1+)'	9.5524(9)	12.5921(12)	5.1876(5)	90	90	90	623.99
DEPJIR	'(C6 H14 N4 O8 Zn2 2+)n,2n(C1 H1 O2 1-)'	11.617(10)	8.717(3)	8.289(2)	90	90	90	839.39
DEPJIR01	'(C3 H3 O6 Zn1 1-)n,n(C1 H5 N2 1+)'	8.717(3)	11.617(10)	8.289(2)	90	90	90	839.39
DEWHET	'(C4 H10 N2 O3 S1 Zn1)n'	7.32690(10)	8.29220(10)	12.1221(2)	90	90	90	736.49
DEWXUY	'(C6 H12 Cl2 N4 Zn1)n'	11.680(4)	6.857(4)	6.011(4)	90	90	90	481.42
DEWYAF	'(C6 H12 Br2 N4 Zn1)n'	11.889(6)	7.215(5)	6.023(4)	90	90	90	516.65
DITTAC	'(C4 H4 Br2 N2 Zn1)n'	12.2327(14)	3.7481(3)	7.2659(6)	90	90	90	333.14
DOPYAJ	'(C6 H8 Cl2 N2 Zn1)n'	6.0621(4)	10.2156(8)	13.9518(8)	90	90	90	864.01
DOPYIR	'(C6 H8 Br2 N2 Zn1)n'	6.2698(6)	10.3167(7)	14.3842(9)	90	90	90	930.42
DUWTOG	'(C5 H8 N8 O2 Zn2)n'	14.102(13)	10.140(9)	6.842(6)	90	90	90	978.37
ECIHIK	'(C8 H12 N10 O4 Zn1)n'	12.534(3)	6.5368(13)	8.5337(17)	90	90	90	699.19
ECOLOZ	'(C5 H6 N4 O2 Zn1)n'	15.882(3)	4.7671(9)	9.9959(19)	90	90	90	756.80
EGEBIC	'(C3 H5 N1 O2 S1 Zn1)n'	6.025(3)	8.838(5)	9.402(5)	90	90	90	500.65
EVUWIB	'(C4 H9 N2 O6 P1 Zn1)n'	5.0349(2)	9.4539(4)	18.6092(8)	90	90	90	885.79
EYUZUU01	'(C8 H10 N6 O4 Zn2)n'	9.2729(18)	8.3720(17)	8.1317(17)	90	90	90	631.29
FEBMUV	'(C7 H7 N1 O6 Zn1)n,n(H2 O1)'	7.3509(2)	9.4432(3)	13.8586(2)	90	90	90	962.01
FIQBOW	'(C8 H8 Cl2 O1 Zn1)n'	7.1310(10)	21.012(4)	6.4700(10)	90	90	90	969.44
FIRGIW	'(C4 H6 Cl1 N1 O4 Zn1)n'	8.556(1)	8.566(1)	9.804(1)	90	90	90	718.54
FUDQIF	'(C8 H8 F6 N4 Si1 Zn1)n'	7.1409(10)	7.1409(10)	7.6068(15)	90	90	90	387.89
GAYFOD	'(C6 H4 N4 Zn1)n,n(C3 H7 N1 O1)'	8.8312(19)	8.8312(19)	7.3007(23)	90	90	90	569.38
GIBWOE	'(C10 H2 O8 Zn2)n'	16.611(3)	7.4280(14)	8.0376(16)	90	90.496(3)	90	991.69
GICXIB	'(C3 H3 O6 Zn1 1-)n,C3 H8 N1 1+'	8.552(3)	12.027(4)	8.696(3)	90	90	90	894.43
GUTRET	'(C4 H4 N4 P2 Zn1)n'	8.15939(14)	14.48130(33)	7.32262(14)	90	90	90	865.23
HABDEU01	'(C14 H14 N2 O4 S1 Zn1)n'	8.2546(7)	6.9145(6)	13.3739(11)	90	90	90	763.33
HAXFIV	'(C4 N6 Zn1)n'	7.6070(3)	7.5828(4)	11.8468(6)	90	90	90	683.35
HEDNOT	'(C7 H12 O7 Zn2)n'	12.468(4)	7.801(2)	6.105(1)	90	90	90	593.79
HERYOT	'(C14 H8 O10 Zn2)n'	9.773044(23)	7.060516(17)	9.879739(22)	90	90	90	681.73
HESVOR	'(C14 H4 N2 O8 Zn2)n,n(H2 O1)'	7.0649(4)	7.0649(4)	19.775(2)	90	90	90	987.03
HEWPIJ	'(C1 H6 N1 1+)n,n(C3 H3 O6 Zn1 1-)'	8.4127(8)	11.7270(10)	8.1080(8)	90	90	90	799.90
HIQPII	'(C10 H12 N4 Zn1)n'	8.81181(53)	8.81181(53)	7.36675(47)	90	90	90	572.01
HOYQAP	'(C9 H10 N4 O3 Zn2)n'	10.536(9)	12.314(10)	4.659(4)	90	90	90	604.46
HUPRUF01	'(C1 H3 N5 O1 Zn1)n'	6.3449(5)	10.4301(7)	6.6211(5)	90	90	90	438.17

IBOSUN	'(C3 H5 N2 O4 P1 Zn1)n'	5.1971(6)	7.6972(9)	17.336(2)	90	90.618(2)	90	693.45
IGOYOU	'(C8 H6 N6 O1 Zn1)n'	5.3812(3)	11.9615(5)	15.3812(9)	90	90	90	990.05
IVAZUA	'(C7 H3 N1 O4 Zn1)n'	8.4225(17)	6.5742(13)	12.899(3)	90	90	90	714.23
IYEXEP	'(C12 H8 O6 Zn2)n'	11.9703(7)	7.8154(5)	6.2428(4)	90	90.816(2)	90	583.97
JAHGAA	'(C6 H7 O4 P1 Zn1)n'	5.634(2)	14.339(5)	4.833(1)	90	90	90	390.44
JIHROH	'(C8 N6 Zn1)n'	7.466(2)	5.3171(5)	10.482(2)	90	90	90	416.11
KAMDIL	'(C8 H16 Cl4 O2 Zn2)n'	6.928(1)	7.306(1)	15.197(3)	90	90	90	769.21
KEKLIY	'(C3 H6 N1 O6 P1 Zn1)n'	5.1818(6)	7.6909(9)	17.7166(15)	90	90	90	706.05
KIJKOE	'(C5 H6 Cl2 N1 O3 P1 Zn1)n'	8.497(5)	9.391(5)	12.378(6)	90	90.860(11)	90	987.60
KOQZAT	'(C3 H10 B4 N2 O7 Zn1)n'	8.670(4)	8.670(4)	12.722(13)	90	90	90	956.30
LARQIF	'(C4 H12 N2 O4 Zn1 2+)n,n(C8 H4 O4 2-)'	9.4920(5)	10.3825(3)	7.2533(3)	90	90	90	714.82
LERSAE	'(C16 H17 Cl1 N4 O2 Zn1)n'	7.4510(5)	14.1636(8)	8.1977(5)	90	90.459(6)	90	865.10
LIHBUB	'(C10 H7 N3 O5 Zn1)n'	6.6828(8)	8.4311(10)	17.722(2)	90	90	90	998.52
LIHRIE	'(C2 H3 N3 O5 S1 Zn2)n'	7.3183(4)	6.8119(4)	13.7846(7)	90	90	90	687.18
LOQFEE	'(C8 H7 N1 O6 Zn1)n'	16.9663(13)	10.8788(8)	4.9606(4)	90	90	90	915.59
LUCREH	'(C7 H3 N1 O4 Zn1)n'	6.730(3)	14.156(6)	7.299(3)	90	90	90	695.38
LUGLUU	'(C12 H8 Cl2 N10 Zn2)n'	6.7191(5)	14.0805(11)	9.0468(7)	90	90.600(2)	90	855.86
LUZYUA	'(C2 H8 N2 S2 Zn2)n'	17.26305(32)	6.39336(11)	6.20451(10)	90	90	90	684.79
MAHPUG	'(C12 H8 N2 O4 Zn1)n'	5.3780(11)	10.967(2)	11.443(2)	90	90	90	674.91
MAPCOV	'(C6 H6 N4 Zn1)n'	7.4829(4)	14.3844(6)	7.3831(3)	90	90	90	794.70
MICDUX	'(C2 H8 N2 Se2 Zn2)n'	6.6298(9)	6.4608(9)	17.350(2)	90	90	90	743.17
MICFAF	'(C3 H10 N2 Se2 Zn2)n'	19.9731(18)	6.6268(7)	6.4394(6)	90	90	90	852.30
MUJGII	'(C12 H12 Cu2 N8 Zn1)n'	10.9623(3)	10.9623(3)	6.3231(4)	90	90	90	759.86
MUQVEA	'(C2 H9 B1 Cl1 N11 Zn1)n,n(H2 O1)'	9.4283(5)	5.0074(2)	12.3291(6)	90	90	90	582.07
NAHNLB01	'(Na1 1+)n,n(C6 H6 N1 O6 Zn1 1-),n(H2 O1)'	7.869(4)	9.783(6)	12.292(6)	90	90	90	946.27
NASCAN	'(C3 H10 N2 S2 Zn2)n'	19.899	6.398	6.1951	90	90	90	788.72
NAZGON	'(C10 H8 Cl2 N2 Zn1)n'	11.9267(7)	11.3884(6)	3.62444(17)	90	90	90	492.29
NIPWIT	'(C7 H5 N1 O6 Zn2)n'	7.7477(8)	18.698(2)	5.7744(6)	90	90	90	836.52
NIQREK	'(C4 H6 O6 Zn1)n'	5.725(1)	16.251(2)	6.825(1)	90	90.72(1)	90	634.93
NUXMIC01	'(C3 H6 O6 P2 Zn2)n'	8.4886(6)	18.8650(10)	5.2720(4)	90	90	90	844.25
ODIVON	'(C20 H16 N6 O4 Zn1)n'	10.0177(14)	16.292(2)	5.9802(9)	90	90	90	976.02
ODOJAT	'(C2 H5 Na1 O6 P2 Zn1)n'	5.2813(5)	16.227(2)	8.5998(10)	90	90.732(5)	90	736.94
OFIXOR	'(C10 H7 N1 O3 Zn1)n'	10.790(6)	17.585(10)	5.148(3)	90	90	90	976.79
OLUZUR	'(C2 H3 Al1 F5 N3 Zn1)n'	8.92885(3)	7.098858(20)	9.25930(3)	90	90	90	586.90
OQOMAK	'(C1 H5 F2 N5 O1 Zn1)n'	6.2611(6)	6.9066(5)	13.6068(13)	90	90	90	588.40
PEYGAC	'(C2 H4 Cl2 N4 Zn1)n'	13.6756(8)	7.3710(5)	7.4200(5)	90	90	90	747.96
PIPKUW	'(C9 H8 N2 S1 Zn1)n'	9.7372(8)	12.7543(16)	7.4397(7)	90	90	90	923.95
POYRUR	'(C6 H8 O8 Zn1)n'	5.9314(4)	10.3966(6)	13.4315(8)	90	90	90	828.27
PUBGID	'(C18 H16 N2 O6 Zn1)n'	17.8339(14)	6.4682(5)	7.4305(6)	90	90.795(8)	90	857.05
PYZNDT	'(C5 H5 N1 O4 S2 Zn1)n'	8.493(2)	11.095(3)	9.161(2)	90	90	90	863.24
QENFUL	'(C12 H14 N6 O8 Zn1)n'	8.8184(18)	12.627(3)	7.4326(15)	90	90.86(3)	90	827.53
QITBEC	'(C8 H12 N2 O4 S1 Zn1)n'	9.8004(4)	10.7829(3)	4.88473(19)	90	90	90	516.20
QOBHEU	'(C2 H8 N2 Te2 Zn2)n'	5.660(1)	17.156(3)	4.336(1)	90	90	90	421.04
QOBHEU01	'(C2 H8 N2 Te2 Zn2)n'	7.061(1)	6.927(1)	17.524(4)	90	90	90	857.13
QOBHIY	'(C3 H10 N2 Te2 Zn2)n'	20.169(4)	7.038(1)	6.882(1)	90	90	90	976.90
QOGJIF	'(C8 H6 O5 Zn1)n'	8.3887(6)	6.0883(5)	16.8795(10)	90	90	90	862.09
QOTZOP	'(C8 H10 O4 Zn1)n'	4.8436(2)	6.6125(3)	26.2382(13)	90	90	90	840.37

ROSKIV	'(C9 H6 N4 O2 Zn1)n'	18.5081(5)	4.82300(10)	10.9635(4)	90	90	90	978.65
ROSKOB	'(C9 H6 N4 O2 Zn1)n'	10.4858(3)	18.8309(6)	4.8130(2)	90	90	90	950.36
RUMRUO	'(C4 H8 F5 N20 Zn4 1-)n,C2 H8 N1 1+'	6.5576(4)	9.7150(6)	8.6358(6)	90	90.579(4)	90	550.13
SANBOZ	'(C12 H20 N4 O10 Zn2)n'	7.6130(11)	15.736(2)	6.9581(10)	90	90	90	833.57
SIJREJ	'(C7 H5 N1 O6 Zn1)n'	5.8976(5)	5.8184(5)	23.7875(19)	90	90.5730(10)	90	816.22
SIWQIA	'(C3 H3 O6 Zn1 1-)n,H5 N2 1+'	8.6640(3)	7.7157(2)	11.4824(4)	90	90	90	767.59
SIYSAV	'(C7 H8 Cl1 N1 O1 Zn1)n'	5.0670(6)	9.1795(10)	18.293(2)	90	90	90	850.85
TACSIB	'(C3 H7 Cl2 N1 O2 Zn1)n'	6.9371(14)	12.918(3)	7.9596(16)	90	90	90	713.29
TISLAJ	'(C6 H4 N6 O4 Zn2)n'	9.7119(8)	7.6320(5)	13.4698(10)	90	90	90	998.40
TISTAQ	'(C4 H4 Cl2 N2 Zn1)n'	7.127(1)	12.057(3)	3.564(1)	90	90	90	306.26
TISTEU	'(C4 H4 Cl2 N2 Zn1)n'	3.576(1)	7.066(4)	12.169(1)	90	90	90	307.49
TOJVUJ	'(C6 H8 O8 P2 Zn2)n'	19.2991(6)	4.8232(2)	5.6545(2)	90	90	90	526.34
UBOBES	'(C10 H6 Cl6 N2 Zn1)n'	13.846(3)	13.846(3)	3.6542(10)	90	90	90	700.55
UBOBIW	'(C10 H6 Br4 Cl2 N2 Zn1)n'	13.888(3)	13.888(3)	3.7300(12)	90	90	90	719.43
UBOCIX06	'(C10 H8 Cl2 N2 Zn1)n'	11.380(2)	11.922(2)	3.6199(6)	90	90	90	491.12
VADQAS	'(C12 H12 O8 P2 Zn2)n'	27.904(1)	4.8273(3)	5.6450(2)	90	90	90	760.39
VAGJAP	'(C2 H4 N1 O4 P1 Zn1)n,n(H2 O1)'	9.5560(13)	12.611(2)	5.2318(8)	90	90	90	630.49
VAHWIM	'(C8 H4 N8 Zn1)n'	8.1103(6)	8.7455(8)	13.0119(10)	90	90	90	922.92
VAMWEM	'(C4 H12 N2 Se2 Zn2)n'	6.6407(30)	6.4668(29)	22.299(10)	90	90	90	957.61
VERZUP	'(C3 H3 O6 Zn1 1-)n,n(H4 N1 O1 1+)'	7.6892(2)	7.7385(2)	13.0205(4)	90	90	90	774.76
VERZUP01	'(C3 H3 O6 Zn1 1-)n,n(H4 N1 O1 1+)'	8.61779(12)	7.73073(10)	11.50052(16)	90	90	90	766.19
VESNEP	'(C12 H16 O8 Zn2)n'	16.2037(17)	4.7810(2)	9.2692(6)	90	90.329(7)	90	718.07
VIHWIS	'(C8 H6 N4 O2 Zn1)n'	7.39188(21)	7.39188(21)	17.3389(6)	90	90	90	947.40
WAFPUP	'(C6 H12 Cl2 N2 Zn1)n'	6.6061(17)	11.5023(18)	11.680(2)	90	90	90	887.51
WAVDUT	'(C2 H2 O6 P1 Zn1 1-)n,n(H4 N1 1+)'	10.245(2)	12.447(3)	5.1538(11)	90	90	90	657.21
WOBFIE	'(C2 H2 O5 Zn1)n'	6.1672(3)	9.4030(5)	15.1739(8)	90	90	90	879.94
WURWUD	'(C6 H6 O6 S1 Zn1)n'	4.974(2)	12.000(6)	14.514(7)	90	90	90	866.31
XAJZAK	'(C2 H2 O5 P1 Zn1 1-)n,n(H4 N1 1+)'	9.5324(13)	12.5898(17)	5.1920(7)	90	90	90	623.10
XALXIS	'(C6 H4 N4 O2 Zn1)n'	5.995(4)	10.540(4)	12.586(6)	90	90	90	795.28
XANZES	'(C4 H7 N2 O3 P1 Zn1)n'	5.2488(5)	9.6411(8)	14.5214(13)	90	90	90	734.84
XATNIP	'(C10 H12 O8 Zn2)n'	13.933(2)	4.7820(10)	9.281(2)	90	90.620(10)	90	618.34
YAVGEJ	'(C6 H8 O8 Zn1)n'	7.3677(15)	8.1353(16)	15.107(3)	90	90	90	905.49
YEJXIW	'(C3 H8 N1 O3 P1 Zn1)n,n(H2 O1)'	9.09424(16)	5.011819(67)	16.06675(35)	90	90.3819(16)	90	732.29
YEJXUI	'(C4 H10 N1 O3 P1 Zn1)n'	8.57047(66)	8.37815(40)	9.90161(57)	90	90.9437(46)	90	710.89
YOBNAG	'(C12 H22 N4 O8 Zn1)n,n(C1 H4 O1),0.5n(H2 O1)'	13.6542(6)	14.8585(6)	4.7251(2)	90	90	90	958.63
YOBPOW	'(C10 H18 N4 O8 Zn1)n,0.666n(C1 H4 O1),0.33n(H2 O1)'	13.8742(6)	14.6060(7)	4.7321(2)	90	90	90	958.94
YOBPUC	'(C10 H18 N4 O8 Zn1)n,1.67n(C1 H4 O1),n(H2 O1)'	14.0129(10)	14.6036(10)	4.7205(3)	90	90	90	966.00
YUKVUW	'(C3 H3 O6 Zn1 1-)n,n(C1 H6 N3 1+)'	8.3493(3)	11.7276(5)	8.9089(4)	90	90	90	872.34
ZNAASP01	'(C4 H9 N1 O6 Zn1)n,n(H2 O1)'	9.443(5)	7.862(4)	11.696(6)	90	90	90	868.32
ZNGLUD	'(C5 H9 N1 O5 Zn1)n,n(H2 O1)'	11.190(2)	10.463(1)	7.220(2)	90	90	90	845.33
ZUBZIH	'(C6 H10 N2 O4 S2 Zn1)n'	20.1581(3)	9.61834(15)	5.03695(8)	90	90	90	976.60

Table S2. DS2 MOF structures. Pore diameters, a/b/c and volume are given in Å. Angles in °.

CSD code	Chemical composition	a	b	c	alpha	beta	gamma	volume	pore
ASINAT	'(C93 H65 N9 O13 Zn3)n,18n(C3 H7 N1 O1),3n(H2 O1)'	21.007(4)	21.099(4)	21.240(4)	63.477(3)	63.691(2)	84.660(3)	7486.03	9.25
ATAHUA	'(C70 H48 Cd3 N8 O12)n,3n(H2 O1)'	11.6274(18)	19.663(4)	32.678(6)	90	90	90	7471.16	5.41
BEDMOO	'(C28 H20 F6 N4 O4 Zn1)n,n(H2 O1)'	21.3188(14)	17.1245(11)	21.1963(13)	90	90	90	7738.21	5.81
CABJEX	'(C30 H20 N12 O16 S4 Zn4)n'	20.1368(10)	20.2976(8)	17.4633(12)	90	90	90	7137.75	7.77
CAVRAU	'(C36 H31 N9 O13 Zn5)n,n(C3 H7 N1 O1),n(H2 O1)'	15.508(11)	19.220(13)	25.211(17)	90	90	90	7514.49	7.75
CAVREY	'(C36 H31 N9 O16 Zn5)n,n(C3 H7 N1 O1),5n(H2 O1)'	15.585(4)	19.237(5)	25.305(7)	90	90	90	7586.66	6.20
CUBBEI	'(C42 H34 O12 Zn3)n'	18.1019(8)	18.1019(8)	24.668(2)	90	90	120	7000.24	11.32
DEVWOT	'(C58 H46 N4 O16 Zn2)n,7(H2 O1),C3 H7 N1 O1'	21.2932(8)	20.9091(6)	16.9902(6)	90	111.641(4)	90	7031.21	5.89
ECOWUQ	'(C42 H27 N3 O6 Zn2)n'	21.253(2)	37.539(3)	9.3861(14)	90	93.753(11)	90	7472.33	13.22
EMITOK	'(C24 H16 Cd1 N2 O6 S1)n'	18.5317(8)	16.6605(6)	22.9353(7)	90	94.289(3)	90	7061.38	6.07
EWOVET	'(C52 H34 N12 O8 Zn3)n,8(C4 H9 N1 O1)'	21.027(2)	21.027(2)	20.5274(10)	90	90	120	7859.94	8.51
FANPAO	'(C36 H20 N20 O16 Zn4)n,C3 H7 N1 O1,2(H2 O1)'	17.8735(9)	20.9554(14)	20.7462(13)	90	90	90	7770.41	5.76
FAYPIG	'(C75 H60 N18 O12 Zn5)n,n(H2 O1)'	19.562(4)	20.850(2)	23.5730(12)	115.321(1)	112.654(1)	92.849(2)	7750.9	11.51
FEHCOM	'(C24 H20 N4 O4 Zn2)n'	13.9249(12)	23.653(2)	23.637(2)	90	90	90	7785.22	7.42
GATJIV	'(C68 H56 Cd1 Cl4 N4 O6 2+)n,2n(Cl1 O4 1-),2n(C3 H7 N1 O1),3n(C2 H6 O1),1.67n(H2 O1)'	26.209(2)	26.209(2)	12.7517(16)	90	90	120	7585.77	6.35
GEXPAD	'(C120 H84 Cd6 N12 O36 S6)n,2(C4 H8 O2),4(H2 O1)'	12.161(2)	23.730(4)	25.540(4)	90	91.723(3)	90	7367.01	5.23
GUKPEJ	'(C24 H26 N4 O16 Zn3)n,2n(H2 O1)'	24.4473(9)	24.4473(9)	14.0673(15)	90	90	120	7281.2	5.51
GULWOA	'(C30 H34 Cd5 Cl6 N22 O4)n,10n(C3 H7 N1 O1)'	29.728(5)	12.530(2)	20.920(4)	90	114.847(4)	90	7071.2	6.47
GUPBOJ01	'(C48 H60 Cd6 N24)n'	16.9693(17)	29.411(3)	14.6756(15)	90	103.622(2)	90	7118.33	5.55
HAJKIO	'(C12 H10 Cd1 N4 O4)n'	12.869(5)	23.643(10)	24.900(11)	90	90	90	7576.12	6.67
HUQGOR	'(C93 H65 N5 O13 Zn3)n'	19.792(5)	20.604(5)	21.471(6)	115.799(6)	98.322(7)	100.882(7)	7482.02	9.66
HUQHAE	'(C94 H67 N5 O13 Zn3)n'	19.608(4)	21.133(4)	21.571(4)	117.428(3)	100.548(4)	99.067(3)	7493.93	9.25
HURFUX	'(C36 H34 N12 O13 Zn5)n,n(C3 H7 N1 O1),n(H2 O1)'	15.4115(16)	19.185(2)	25.471(3)	90	90	90	7531	6.75
HUZFOY	'(C78 H54 Cd1 N12 2+)n,2n(Cl1 O4 1-)'	21.545(2)	21.545(2)	19.137(3)	90	90	120	7693.03	6.01
IQOJEF	'(C124 H84 N16 O16 Zn4)n,4n(H2 O1),4n(C3 H7 N1 O1)'	14.2232(7)	26.5395(14)	19.4670(10)	90	107.7010(10)	90	7000.44	6.30
JABGUR	'(C15 H18 N14 O1 Zn2)n,C3 H7 N1 O1'	25.3735(9)	25.3735(9)	12.8546(6)	90	90	120	7167.21	7.04
JENROM	'(C88 H58 N4 O13 Zn3)n'	18.2797(7)	21.2557(6)	21.7570(8)	61.587(3)	78.504(4)	82.525(3)	7280.05	10.55
KUYGOC	'(C96 H60 Cd4 O24)n,13(C3 H7 N1 O1),6(C2 H6 O1)'	43.6263(18)	13.2340(7)	13.8249(7)	90	108.465(3)	90	7570.89	8.25
LUMDEC	'(C24 H20 Cd2 N8 O8)n,n(H2 O1)'	18.569(3)	18.569(3)	23.042(2)	90	90	90	7945.06	5.61
LUMDIG	'(C12 H10 Cd1 N4 O4)n'	18.569(3)	18.569(3)	23.015(1)	90	90	90	7935.75	7.91
MUQSAU	'(C28 H20 N2 O10 Zn2)n'	29.647(6)	24.669(5)	9.7421(19)	90	90	90	7125	6.11
NATHUO	'(C48 H18 F18 O12 Zn2 2-)n,2(C2 H8 N1 1+)'	7.8849(2)	36.8328(7)	26.7656(5)	90	90	90	7773.34	7.57
OFEHAK	'(C12 H10 Cd1 N2 O5)n,0.25n(H2 O1)'	22.290(3)	22.290(3)	15.123(3)	90	90	90	7513.77	5.48
OFEHEO	'(C34 H24 Cd2 N6 O8)n'	22.143(4)	22.143(4)	16.282(6)	90	90	90	7983.27	5.41
OHAPAQ	'(C60 H54 N10 O8 Zn2)n,C3 H7 N1 O1,4(H2 O1)'	16.668(6)	16.256(6)	28.596(10)	90	90	90	7748.23	6.09
OLEYAH	'(C8 H2 O6 Zn2)n'	22.9556(13)	22.9556(13)	15.883(2)	90	90	120	7248.37	9.34
OPOBIF	'(C13 H10 N6 O4 Zn2)n,n(H2 O1)'	32.8723(16)	32.8723(16)	8.4085(8)	90	90	120	7868.82	6.22
PEKTUW	'(C28 H18 N2 O5 S1 Zn1)n'	20.682(3)	19.366(3)	20.733(3)	90	114.878(2)	90	7533.56	7.98
PEMRIK	'(C28 H17 N5 O8 Zn2)n,n(C5 H11 N1 O1),0.5n(H2 O1)'	34.6925(7)	16.6027(4)	13.7633(3)	90	105.3030(10)	90	7646.43	6.09

PEQKUT	'(C68 H48 Cd1 N12 O18 P6)n,n(C1 H2 Cl2)'	31.874(5)	11.337(5)	21.874(5)	90	90	90	7904.29	5.03
PUGSER	'(C32 H17 O15 Zn4 1-)n,n(C2 H8 N1 1+)'	10.316(2)	26.096(5)	27.889(6)	90	93.78(3)	90	7491.56	9.41
PUGSIV	'(C68 H32 O30 Zn8 2-)n,2n(C2 H8 N1 1+)'	10.306(2)	27.776(6)	26.232(5)	90	91.84(3)	90	7505.29	9.70
PUGSOB	'(C72 H34 O30 Zn8 2-)n,2n(C2 H8 N1 1+)'	10.327(2)	26.237(5)	27.756(6)	90	93.83(3)	90	7503.68	9.48
PUGSUH	'(C72 H34 O30 Zn8 2-)n,2n(C2 H8 N1 1+)'	10.364(2)	26.746(5)	27.804(6)	90	93.91(3)	90	7689.21	9.31
PUSXIL	'(C16 H6 O14 P2 Zn3 2-)n,2n(H3 O1 1+)'	18.310(6)	18.310(6)	23.222(11)	90	90	90	7785.32	6.90
QAFJEP	'(C64 H50 Cd2 N14 O10)n,4(H2 O1)'	33.07(3)	10.122(9)	21.692(19)	90	98.40(2)	90	7183.17	5.27
QOJBAU	'(C108 H56 Cl8 F20 N12 Zn4)n'	14.3665(6)	20.7814(8)	26.2162(13)	99.654(3)	97.510(3)	103.905(3)	7369.49	6.51
RUCSEP	'(C46 H32 N2 O28 P4 Zn6)n,12n(H2 O1)'	41.255(2)	8.4745(5)	20.7206(13)	90	96.0520(15)	90	7203.87	5.93
RUGXIC	'(C16 H9 O11 Zn2 1-)n,n(C2 H8 N1 1+),3.25n(C3 H7 N1 O1)'	23.6519(17)	13.0546(9)	26.4620(19)	90	115.424(3)	90	7379.29	5.77
SAKSOO	'(C2 H8 N1 1+)n,n(C27 H21 Cd1 N6 O6 1-),n(H2 O1)'	29.28(2)	14.524(10)	20.084(15)	90	115.414(11)	90	7714.47	5.72
SARNOQ	'(C4 H1 N11 Zn1)n,n(C4 H9 N1 O1)'	23.8620(19)	23.8620(19)	14.6860(19)	90	90	120	7241.82	6.70
SERWAP	'(C176 H192 F24 N16 O32 Si4 Zn4)n,4n(C1 H1 Cl3)'	22.0440(15)	22.0440(15)	15.1513(18)	90	90	90	7362.59	5.42
TELDOF	'(C18 H15 Cd1 N3 O4)n'	22.425(5)	22.425(5)	15.091(10)	90	90	90	7588.97	5.80
TUKDEK	'(C24 H18 Cd1 N6 O4)n,11n(H2 O1)'	13.8290(5)	20.2540(8)	25.7650(10)	90	90	90	7216.58	6.38
TULLIX	'(C42 H36 Cd3 O23)n'	46.561(7)	5.9263(9)	33.495(6)	90	128.794(2)	90	7203.58	7.94
VEXQIA	'(C50 H62 Cl1 K2 N20 O11 1+)n,n(H2 Cl3 O1 Zn1 1-),24n(H2 O1)'	16.354(3)	24.747(5)	19.137(4)	90	112.85(3)	90	7137.19	6.31
VULWEF	'(C33 H20 N2 O10 Zn2)n,2n(C3 H7 N1 O1),n(H2 O1)'	21.889(5)	10.156(5)	34.909(5)	90	90.715(5)	90	7759.83	5.00
WARFAZ	'(C30 H22 Cd1 N4 O9)n,0.5(C3 H7 N1 O1),3.5(H2 O1)'	21.838(3)	21.838(3)	14.721(3)	90	90	90	7020.42	5.30
WEDSIK	'(C78 H66 Cd3 N12 O20 P2)n,3(H2 O1)'	16.783(8)	16.783(8)	30.325(17)	90	90	120	7397.26	6.50
WITWIH	'(C30 H18 N4 O8 Zn1)n,0.5n(C4 H8 O1),0.5n(C1 H4 O1),0.25n(H2 O1)'	22.3598(7)	15.1429(4)	23.0395(7)	90	110.657(4)	90	7299.46	5.81
WOMCUY	'(C32 H18 Cd2 Cl2 N6 O8)n'	22.0734(10)	22.0734(10)	16.1233(14)	90	90	90	7855.84	5.30
WONZUV	'(C32 H24 F6 N4 Si1 Zn1)n,n(C1 H1 Cl3),n(H2 O1)'	22.0593(13)	22.0593(13)	15.0937(18)	90	90	90	7344.79	11.46
WORTAA	'(C54 H46 B2 Cd2 F4 N6 O8)n'	21.466(4)	21.361(4)	16.675(3)	90	97.83(3)	90	7574.79	7.08
WUZGAB	'(C176 H120 Cd6 O48 4-)n,2n(H10 Ca1 O5 2+)'	15.631(5)	18.456(6)	27.517(10)	80.164(7)	89.994(7)	76.264(6)	7591.09	8.28
XEJJII	'(C40 H24 N4 O10 Se2 Zn2)n'	17.124(3)	30.169(6)	14.903(3)	90	90	90	7699.1	7.12
XEZNEY	'(C10 H9 N3 O2 Zn1)n'	27.5934(13)	27.5934(13)	10.7913(4)	90	90	120	7115.65	6.93
XOVZEO	'(C72 H56 N16 Zn2 4+)n,4n(C1 F3 O3 S1 1-),n(C4 H8 O2),n(C2 H6 O1 S1),n(H2 O1)'	21.111(3)	17.542(3)	21.355(3)	90	97.37(3)	90	7843.04	5.86
XUTMAC	'(C32 H23 Cd2 N13 O6)n'	29.1344(11)	8.6686(3)	31.9584(14)	90	112.448(5)	90	7459.65	5.33
XUVQOW	'(C56 H42 Cd4 N2 O29 2-)n,2(C2 H8 N1 1+)'	18.633(5)	20.399(5)	20.852(5)	90	90	90	7925.73	5.29
YEKHUU	'(C43 H49 N7 O13 Zn2)n'	14.232(5)	20.366(7)	26.441(9)	90	90.884(13)	90	7662.98	9.52
YEKJEG	'(C43 H49 Cd2 N7 O13)n'	14.730(3)	28.473(7)	18.577(5)	90	90	90	7791.33	9.83
ZEHJEE	'(C22 H24 N2 O8 Zn2)n,x(C4 H9 N1 O1),x(C2 H6 O1),x(H2 O1)'	36.5943(12)	36.5943(12)	6.7186(2)	90	90	120	7791.77	11.41
ZUCGAH	'(C80 H70 N4 P2 S2 Zn1)n'	28.4395(15)	18.7648(11)	16.3621(9)	90	123.051(3)	90	7318.89	5.16

Table S3. DS1 structures band gap evaluation at PBE level computed at Γ (u) and using 2x2x2 k-point (k2) sampling. All values are given in eV. Cell volume is given in $Å^3$.

	HOMO u	LUMO u	HOMO k2	LUMO k2	band gap u	band gap k2	difference	cell volume
ASALEL	1.25	4.24	1.41	3.88	2.99	2.48	0.51	5616
BENKOW	1.84	6.83	1.86	6.83	4.99	4.97	0.02	4362
BENQUH	2.05	6.63	2.15	6.64	4.58	4.50	0.09	4858
BUKJIA	1.29	4.13	1.31	4.09	2.84	2.79	0.05	3448
BUWLEL01	-1.10	3.50	-0.93	3.50	4.59	4.43	0.16	6605
CAKLOR	0.80	5.83	0.86	5.70	5.03	4.84	0.19	4823
CAVQOH	2.44	6.87	2.52	6.87	4.43	4.35	0.08	5211
CIMFIP	1.05	4.18	1.86	3.90	3.13	2.05	1.08	4729
CIMZII	2.13	6.85	2.27	6.85	4.72	4.58	0.14	4164
CUJBAK01	0.47	5.11	0.47	5.12	4.65	4.64	0.00	5433
CUMBAO	1.89	6.74	1.89	6.55	4.86	4.65	0.20	4894
DASLOZ	1.72	4.22	1.73	4.23	2.50	2.50	0.00	6673
DEHYEV	1.57	6.21	1.58	6.22	4.64	4.64	0.01	4211
DEPJIR	1.21	4.78	1.24	4.74	3.57	3.50	0.07	5664
DEPJIR01	1.42	5.55	1.41	5.55	4.13	4.14	-0.01	5664
DEWHET	2.90	7.31	2.92	7.27	4.41	4.35	0.06	4970
DEWXUY	2.94	3.54	3.08	3.49	0.60	0.41	0.19	3249
DEWYAF	2.85	3.45	3.18	3.37	0.59	0.19	0.40	3487
DITTAC	3.44	6.00	3.10	5.13	2.56	2.03	0.54	2248
DOPYAJ	0.94	3.72	0.95	3.73	2.78	2.78	0.01	5831
DOPYIR	1.33	3.62	1.34	3.62	2.29	2.29	0.01	6279
DUWTOG	2.10	6.49	2.05	6.48	4.39	4.43	-0.04	6602
ECIHIK	1.37	5.46	1.35	5.45	4.10	4.10	0.00	4718
ECOLOZ	0.63	5.66	0.82	5.69	5.03	4.87	0.16	5107
EGEBIC	3.39	7.43	3.40	7.44	4.05	4.04	0.01	3379
EVUWIB	1.48	6.65	1.66	6.64	5.17	4.98	0.20	5978
EYUZUU01	1.68	6.07	1.67	6.06	4.39	4.39	0.01	4260
FEBMUV	0.78	3.78	0.77	3.76	3.00	2.99	0.01	6492
FIQBOW	0.44	3.50	0.44	3.43	3.06	2.99	0.07	6542
FIRGIW	1.59	6.45	1.61	6.41	4.86	4.79	0.07	4849
FUDQIF	-0.32	2.27	-0.34	1.97	2.59	2.31	0.29	2618
GAYFOD	-0.59	3.32	-0.61	3.18	3.91	3.79	0.12	3842
GIBWOE	2.59	5.88	2.62	5.88	3.29	3.26	0.03	6692
GICXIB	1.68	5.99	1.67	5.98	4.31	4.31	0.00	6036
GUTRET	1.48	5.15	1.47	5.13	3.66	3.66	0.01	5839
HABDEU01	1.14	3.84	1.15	3.85	2.70	2.69	0.01	5151
HAXFIV	0.53	5.69	0.70	5.36	5.16	4.67	0.49	4611
HEDNOT	0.50	5.13	0.54	5.13	4.63	4.59	0.04	4007
HERYOT	2.77	5.30	2.81	5.30	2.54	2.49	0.04	4600
HESVOR	-0.63	1.92	-0.61	1.87	2.55	2.48	0.07	6661
HEWPIJ	1.28	5.72	1.29	5.73	4.44	4.44	0.00	5398
HIQPII	0.94	5.02	0.95	5.02	4.08	4.07	0.00	3860
HOYQAP	1.64	6.11	2.03	6.11	4.47	4.08	0.39	4079

HUPRUF01	3.28	7.10	3.38	6.90	3.82	3.52	0.30	2957
IBOSUN	1.73	6.30	2.04	6.32	4.57	4.28	0.30	4680
IGOYOU	1.32	4.85	1.34	4.87	3.53	3.53	0.00	6681
IVAZUA	1.96	5.10	1.95	5.10	3.14	3.15	-0.02	4820
IYEXEP	2.29	4.86	2.31	4.79	2.57	2.48	0.09	3941
JAHGAA	1.66	5.88	2.06	5.22	4.22	3.15	1.07	2635
JIHROH	1.91	5.07	2.08	5.09	3.16	3.01	0.15	2808
KAMDIL	0.17	4.39	0.27	4.39	4.23	4.11	0.11	5191
KEKLIY	1.94	6.76	2.05	6.78	4.82	4.73	0.10	4765
KIJKOE	0.98	3.89	0.97	3.89	2.91	2.92	-0.01	6665
KOQZAT	1.87	6.83	1.87	6.83	4.96	4.96	0.00	6453
LARQIF	1.38	3.81	1.36	3.82	2.43	2.45	-0.02	4824
LERSAE	0.94	4.78	0.94	4.75	3.84	3.81	0.03	5838
LIHBUB	2.49	5.37	2.49	5.38	2.88	2.89	-0.01	6738
LIHRIE	3.81	8.18	3.83	8.18	4.37	4.35	0.02	4637
LOQFEE	1.78	5.33	2.02	4.96	3.54	2.94	0.60	6179
LUCREH	1.92	4.90	1.92	4.89	2.98	2.97	0.01	4693
LUGLUU	1.10	4.22	1.10	4.15	3.12	3.05	0.07	5776
LUZYUA	3.60	6.65	3.59	6.66	3.05	3.07	-0.02	4621
MAHPUG	0.87	3.00	0.74	2.96	2.13	2.22	-0.10	4555
MAPCOV	0.70	5.31	0.69	5.31	4.61	4.62	0.00	5363
MICDUX	3.60	6.14	3.58	6.14	2.54	2.57	-0.02	5015
MICFAF	3.25	5.99	3.21	5.98	2.74	2.77	-0.03	5752
MUJGII	2.97	6.41	2.90	6.35	3.44	3.46	-0.02	5128
MUQVEA	0.73	4.92	0.84	4.88	4.19	4.04	0.15	3928
NAHNLB01	2.02	6.07	2.02	6.05	4.05	4.04	0.01	6386
NASCAN	3.27	6.45	3.24	6.45	3.18	3.22	-0.03	5323
NAZGON	2.52	4.46	2.85	4.41	1.94	1.56	0.39	3322
NIPWIT	3.13	5.73	3.14	5.54	2.60	2.41	0.19	5645
NIQREK	1.75	5.41	1.76	5.27	3.66	3.51	0.14	4285
NUXMIC01	2.13	6.60	2.19	6.61	4.47	4.42	0.05	5697
ODIVON	1.15	4.83	1.18	4.51	3.67	3.33	0.35	6587
ODOJAT	2.14	6.99	2.23	7.00	4.85	4.77	0.08	4973
OFIXOR	0.97	4.03	1.17	3.59	3.06	2.41	0.64	6592
OLUZUR	2.57	7.80	2.56	7.79	5.23	5.23	0.00	3961
OQOMAK	2.16	5.92	2.35	5.89	3.76	3.53	0.23	3971
PEYGAC	0.49	5.27	0.52	5.26	4.78	4.74	0.04	5047
PIPKUW	1.73	5.54	1.72	5.43	3.82	3.71	0.11	6235
POYRUR	1.83	6.59	1.83	6.59	4.76	4.76	0.00	5589
PUBGID	1.86	4.18	1.86	4.18	2.32	2.32	0.00	5784
PYZNDT	2.97	5.19	2.98	5.18	2.22	2.20	0.02	5825
QENFUL	1.44	3.30	1.43	3.29	1.86	1.86	0.00	5584
QITBEC	1.62	6.35	2.09	5.69	4.73	3.60	1.13	3483
QOBHEU	4.26	6.24	4.10	6.17	1.98	2.07	-0.09	2841
QOBHEU01	3.56	6.06	3.54	6.05	2.49	2.51	-0.01	5784
QOBHIY	3.21	5.90	3.17	5.89	2.70	2.72	-0.02	6592
QOGJIF	0.89	4.63	0.91	4.47	3.74	3.57	0.17	5818

QOTZOP	1.11	6.03	1.17	5.68	4.92	4.52	0.41	5671
ROSKIV	1.05	5.02	1.55	5.03	3.98	3.48	0.49	6604
ROSKOB	1.31	5.41	1.81	5.30	4.10	3.49	0.61	6413
RUMRUO	2.17	5.71	2.34	5.75	3.54	3.41	0.13	3712
SANBOZ	2.57	6.39	2.55	6.38	3.82	3.83	-0.01	5625
SIJREJ	2.22	5.18	2.22	5.19	2.97	2.96	0.00	5508
SIWQIA	1.49	5.93	1.49	5.88	4.43	4.40	0.03	5180
SIYSAV	0.90	4.45	1.07	4.45	3.55	3.38	0.17	5742
TACSIB	1.47	5.99	1.47	5.98	4.52	4.52	0.00	4814
TISLAJ	2.55	5.93	2.54	5.93	3.38	3.38	0.00	6738
TISTAQ	3.11	5.82	2.73	4.69	2.70	1.96	0.74	2067
TISTEU	3.01	6.15	2.64	5.06	3.14	2.43	0.72	2075
TOJVUJ	2.61	6.74	2.54	6.64	4.13	4.11	0.03	3552
UBOBES	2.33	4.63	3.07	4.55	2.30	1.48	0.82	4728
UBOBIW	2.65	4.98	3.38	4.87	2.33	1.49	0.84	4855
UBOCIX06	2.54	4.62	2.59	4.55	2.08	1.96	0.13	3314
VADQAS	1.88	5.59	2.03	5.54	3.71	3.51	0.20	5131
VAGJAP	1.06	5.60	1.07	5.62	4.54	4.54	0.00	4255
VAHWIM	1.98	5.40	1.97	5.39	3.42	3.42	0.00	6228
VAMWEM	3.05	5.66	3.02	5.66	2.61	2.64	-0.03	6462
VERZUP	1.20	5.69	1.19	5.65	4.48	4.46	0.02	5228
VERZUP01	1.34	5.61	1.36	5.57	4.27	4.21	0.06	5170
VESNEP	0.76	5.90	0.82	5.70	5.14	4.88	0.26	4846
VIHWIS	1.32	4.20	1.53	4.20	2.89	2.67	0.22	6393
WAFPUP	1.56	5.97	1.58	5.97	4.41	4.39	0.02	5989
WAVDUT	2.50	6.86	2.53	6.88	4.36	4.36	0.01	4435
WOBFIE	2.24	5.66	2.23	5.65	3.42	3.41	0.01	5938
WURWUD	1.38	4.97	1.71	4.35	3.58	2.64	0.94	5846
XAJZAK	2.11	6.71	2.16	6.72	4.60	4.56	0.04	4205
XALXIS	1.45	4.56	1.45	4.56	3.11	3.11	0.01	5367
XANZES	1.59	6.60	1.75	6.42	5.01	4.67	0.34	4959
XATNIP	1.26	6.20	1.26	6.03	4.94	4.77	0.17	4173
YAVGEJ	1.16	4.27	1.16	4.27	3.11	3.11	0.00	6111
YEJXIW	0.76	5.33	0.95	5.18	4.57	4.23	0.34	4942
YEJXUI	1.67	6.70	1.67	6.60	5.03	4.93	0.10	4797
YOBNAG	-0.10	4.61	0.19	4.43	4.71	4.24	0.47	6469
YOBPOW	-0.54	3.84	-0.42	3.87	4.39	4.29	0.09	6471
YOBPUC	-0.59	3.81	-0.46	3.84	4.40	4.30	0.10	6519
YUKVUW	1.38	5.87	1.39	5.87	4.49	4.48	0.01	5887
ZNAASP01	1.06	5.81	1.06	5.75	4.75	4.69	0.05	5860
ZNGLUD	0.54	5.35	0.54	5.35	4.80	4.81	0.00	5705
ZUBZIH	2.34	6.87	2.55	4.66	4.53	2.12	2.42	6590

Table S4. Selected **DS1** MOFs band gap evaluation at PBE level with 2x2x2 k-point smapling (k2) and using specific (x x x) sampling (kx). All values are given in eV.

	HOMO k2	LUMO k2	HOMO kx	LUMO kx	k2	kx	(x x x) sampling	difference
ASALEL	1.41	3.88	1.36	4.04	2.48	2.68	**3 2 1**	0.20
CIMFIP	1.86	3.90	1.75	3.94	2.05	2.19	**1 5 2**	0.14
DEWYAF	3.18	3.37	3.18	3.37	0.19	0.19	**1 2 2**	0.01
DITTAC	3.10	5.13	3.04	5.17	2.03	2.13	**1 4 2**	0.10
FUDQIF	-0.34	1.97	-0.34	1.97	2.31	2.31	**2 2 2**	0.00
HAXFIV	0.70	5.36	0.68	5.37	4.67	4.68	**2 2 1**	0.01
HOYQAP	2.03	6.11	1.92	6.11	4.08	4.19	**1 1 3**	0.11
HUPRUF01	3.38	6.90	3.38	6.90	3.52	3.52	**2 1 2**	0.00
IBOSUN	2.04	6.32	2.04	6.32	4.28	4.28	**2 2 1**	0.00
JAHGAA	2.06	5.22	1.77	5.37	3.15	3.60	**3 1 3**	0.45
LOQFEE	2.02	4.96	2.02	4.96	2.94	2.94	**1 2 4**	0.00
NAZGON	2.85	4.41	2.84	4.41	1.56	1.57	**1 1 4**	0.01
ODIVON	1.18	4.51	1.18	4.50	3.33	3.33	**1 1 2**	0.00
OFIXOR	1.17	3.59	1.17	3.59	2.41	2.42	**2 1 4**	0.01
QITBEC	2.09	5.69	2.00	5.75	3.60	3.75	**2 2 5**	0.15
QOTZOP	1.17	5.68	1.16	5.68	4.52	4.52	**5 4 1**	0.01
ROSKIV	1.55	5.03	0.94	4.75	3.48	3.81	**2 1 2**	0.33
ROSKOB	1.81	5.30	1.81	5.30	3.49	3.49	**2 1 4**	0.01
TISTAQ	2.73	4.69	2.67	4.68	1.96	2.01	**2 1 4**	0.04
TISTEU	2.64	5.06	2.58	5.07	2.43	2.49	**4 2 1**	0.07
UBOBES	3.07	4.55	3.04	4.54	1.48	1.49	**1 1 4**	0.01
UBOBIW	3.38	4.87	3.36	4.86	1.49	1.50	**1 1 4**	0.01
VESNEP	0.82	5.70	0.82	5.70	4.88	4.88	**1 4 2**	0.00
WURWUD	1.71	4.35	1.57	4.52	2.64	2.95	**3 1 1**	0.31
XANZES	1.75	6.42	1.77	6.46	4.67	4.70	**3 1 1**	0.02
YEJXIW	0.95	5.18	0.91	5.18	4.23	4.27	**2 3 1**	0.04
YOBNAG	0.19	4.43	0.13	4.52	4.24	4.39	**1 1 3**	0.15
ZUBZIH	2.55	4.66	2.53	4.65	2.12	2.12	**1 2 4**	0.00

Table S5. Selected **DS2** structures band gap evaluation at PBE level computed at Γ (u) and using 2x2x2 k-point (k2) sampling. All values are given in eV. Cell volume is given in Å^3.

	HOMO u	LUMO u	HOMO k2	LUMOk3	band gap u	band gap k2	difference
ATAHUA	0.24	2.63	0.24	2.63	2.38	2.38	0.00
CAVRAU	-1.71	1.45	-1.71	1.45	3.16	3.16	0.00
CAVREY	-1.59	1.53	-1.59	1.53	3.13	3.13	0.00
ECOWUQ	-1.65	0.31	-1.65	0.31	1.96	1.96	0.00
FEHCOM	-1.58	1.45	-1.58	1.45	3.03	3.03	0.00
GATJIV	-0.82	1.27	-0.81	1.26	2.09	2.07	-0.02
GEXPAD	-0.16	2.47	-0.16	2.46	2.63	2.62	-0.01
GUKPEJ	0.93	4.02	0.93	4.02	3.09	3.09	0.00
GULWOA	-1.18	1.87	-1.18	1.87	3.05	3.05	0.00
GUPBOJ	0.28	4.09	0.29	4.09	3.81	3.79	-0.01
HAJKIO	-0.45	2.16	-0.45	2.16	2.62	2.62	0.00
IQOJEF	0.03	2.03	0.03	2.02	1.99	1.99	0.00
JABGUR	-0.34	3.59	-0.34	3.59	3.94	3.93	-0.01
KUYGOC	-1.61	0.69	-1.61	0.69	2.30	2.30	0.00
LUMDIG	-0.85	1.91	-0.85	1.91	2.77	2.77	0.00
MUQSAU	-0.29	1.39	-0.29	1.39	1.68	1.68	0.00
NATHUO	-1.29	1.69	-1.29	1.69	2.98	2.98	0.00
OFEHAK	-1.02	2.05	-1.02	2.05	3.07	3.07	0.00
PEMRIK	-0.82	1.46	-0.82	1.46	2.28	2.28	0.00
PUGSER	-2.53	0.66	-2.53	0.65	3.18	3.17	-0.01
PUGSIV	-2.46	0.27	-2.46	0.28	2.73	2.74	0.01
PUGSOB	-1.84	0.30	-1.83	0.30	2.13	2.13	0.00
PUGSUH	-2.36	0.16	-2.36	0.16	2.51	2.52	0.01
QAFJEP	0.17	2.97	0.17	2.97	2.79	2.80	0.01
QOJBAU	-1.33	1.28	-1.33	1.28	2.62	2.61	0.00
RUCSEP	-0.11	1.85	-0.11	1.84	1.96	1.95	-0.01
RUGXIC	-1.49	0.91	-1.49	0.91	2.40	2.40	0.00
SAKSOO	-0.50	2.54	-0.50	2.54	3.04	3.04	0.00
SERWAP	-1.06	1.58	-1.06	1.58	2.64	2.64	0.00
TELDOF	0.55	3.60	0.55	3.60	3.05	3.05	0.00
TUKDEK	-1.03	1.64	-1.03	1.64	2.67	2.67	0.00
TULLIX	-1.56	1.54	-1.51	1.44	3.10	2.96	-0.14
VEXQIA	1.13	4.32	1.13	4.32	3.19	3.19	0.00
VULWEF	-0.51	1.28	-0.51	1.28	1.80	1.79	0.00
WITWIH	-0.97	1.44	-0.97	1.44	2.41	2.41	0.00
WONZUV	-2.81	-0.19	-2.81	-0.19	2.62	2.62	0.00
WORTAA	-0.86	1.00	-0.85	1.00	1.86	1.86	0.00
WUZGAB	-1.46	1.00	-1.46	1.00	2.46	2.46	0.00
XEJJII	-1.81	-0.14	-1.81	-0.14	1.66	1.66	0.00
XEZNEY	-1.19	1.84	-1.18	1.81	3.02	3.00	-0.03
XUTMAC	1.26	3.41	1.26	3.41	2.15	2.15	0.00
YEKHUU	-1.48	1.11	-1.48	1.11	2.59	2.59	0.00
YEKJEG	-2.10	0.37	-2.10	0.36	2.46	2.46	0.00
ZEHJEE	-0.21	2.40	-0.21	2.32	2.61	2.53	-0.08
ZUCGAH	0.99	2.61	0.99	2.61	1.62	1.62	0.00

Table S6. PBE and PBE0 band gap and S_1 energies (eV) obtained for 36 selected **DS1** MOFs.

	PBE gap	PBE S1	PBE0 gap	PBE0 S1
BUKJIA	2.813	2.824	5.032	3.884
DASLOZ	2.522	2.562	4.708	3.688
DEWXUY	0.653	0.736	3.081	1.485
DOPYAJ	2.811	2.834	4.801	3.794
DOPYIR	2.334	2.363	4.334	3.512
FEBMUV	2.990	3.002	5.311	4.178
FIQBOW	3.063	3.081	4.931	4.056
HABDEU01	2.696	2.701	4.889	3.784
HERYOT	2.529	2.600	4.350	3.438
HESVOR	2.554	2.574	4.791	4.061
IVAZUA	3.114	3.151	5.478	4.448
IYEXEP	2.516	2.677	4.166	3.279
JIHROH	3.161	3.183	5.273	3.917
KIJKOE	3.119	3.135	5.276	4.345
LARQIF	2.467	2.468	4.645	3.635
LIHBUB	2.882	2.903	4.809	3.888
LUCREH	2.986	3.018	5.258	4.252
LUGLUU	3.159	3.162	5.299	4.594
LUZYUA	3.007	3.032	4.904	3.837
MAHPUG	2.126	2.148	4.470	3.548
MICDUX	2.502	2.526	4.277	3.219
MICFAF	2.709	2.727	4.465	3.377
NASCAN	3.153	3.174	5.027	3.933
NIPWIT	2.601	2.612	4.914	4.211
PUBGID	2.317	2.357	3.880	3.165
PYZNDT	2.217	2.300	4.147	3.152
QENFUL	1.855	1.878	4.201	2.905
QOBHEU	1.978	2.007	3.540	2.349
QOBHEU0	2.495	2.507	3.994	2.948
QOBHIY	2.699	2.717	4.145	3.082
SIJREJ	2.967	2.972	5.093	4.069
UBOCIX06	2.081	2.152	4.205	3.782
VAMWEM	2.608	2.628	4.272	3.230
VIHWIS	2.887	2.924	4.7761	3.802
XALXIS	3.113	3.274	5.111	4.232
YAVGEJ	3.109	3.131	4.8875	4.095

Table S7. Computed PBE band gap and PBE0 S_1 values of 36 selected MOFs of **DS1**. The corrected PBE+0.85 values by means of addition of 0.85 eV and their absolute difference with the PBE0 S_1 values is also given, as well as the lowest predicted absorption wavelengths.

	PBE gap (eV)	PBE+0.85 gap (eV)	PBE0 S_1 (eV)	Abs. Diff. (eV)	PBE+0.85 abs (nm)	PBE0 abs (nm)
DEWXUY	0.653	1.503	1.485	0.018	825	835
QOBHEU	1.978	2.828	2.349	0.479	439	528
QENFUL	1.855	2.705	2.905	-0.200	458	427
QOBHEU0	2.495	3.345	2.948	0.397	371	421
QOBHIY	2.699	3.549	3.082	0.467	349	402
PYZNDT	2.217	3.067	3.152	-0.085	404	393
PUBGID	2.317	3.167	3.165	0.002	391	392
MICDUX	2.502	3.352	3.219	0.133	370	385
VAMWEM	2.608	3.458	3.230	0.228	359	384
IYEXEP	2.516	3.366	3.279	0.087	368	378
MICFAF	2.709	3.559	3.377	0.182	348	367
HERYOT	2.529	3.379	3.438	-0.059	367	361
DOPYIR	2.334	3.184	3.512	-0.329	390	353
MAHPUG	2.126	2.976	3.548	-0.572	417	349
LARQIF	2.467	3.317	3.635	-0.318	374	341
DASLOZ	2.522	3.372	3.688	-0.316	368	336
UBOCIX06	2.081	2.931	3.782	-0.851	423	328
HABDEU01	2.696	3.546	3.784	-0.238	350	328
DOPYAJ	2.811	3.661	3.794	-0.133	339	327
VIHWIS	2.887	3.737	3.802	-0.065	332	326
LUZYUA	3.007	3.857	3.837	0.019	322	323
BUKJIA	2.813	3.663	3.884	-0.221	338	319
LIHBUB	2.882	3.732	3.888	-0.156	332	319
JIHROH	3.161	4.011	3.917	0.094	309	317
NASCAN	3.153	4.003	3.933	0.070	310	315
FIQBOW	3.063	3.913	4.056	-0.143	317	306
HESVOR	2.554	3.404	4.061	-0.657	364	305
SIJREJ	2.967	3.817	4.069	-0.252	325	305
YAVGEJ	3.109	3.959	4.095	-0.136	313	303
FEBMUV	2.990	3.840	4.178	-0.338	323	297
NIPWIT	2.601	3.451	4.211	-0.760	359	294
XALXIS	3.113	3.963	4.232	-0.269	313	293
LUCREH	2.986	3.836	4.252	-0.416	323	292
KIJKOE	3.119	3.969	4.345	-0.376	312	285
IVAZUA	3.114	3.964	4.448	-0.484	313	279
LUGLUU	3.159	4.009	4.594	-0.585	309	270

Table S8. Electronic band gap, fermi energy (given as the highest occupied level), electrostatic potential, IP and EA of 20 selected **DS2** computed at PBE and PBE0 level. All in eV.

	PBE					PBE0				
	gap	fermi	work	IP	EA	gap	fermi	work	IP	EA
ASINAT	1.558	-1.713	2.891	-4.604	-3.046	3.052	-2.509	2.903	-5.411	-2.360
CUBBEI	1.768	-2.427	2.452	-4.878	-3.110	3.138	-3.279	2.454	-5.733	-2.595
ECOWUQ	1.996	-2.084	2.707	-4.791	-2.795	3.347	-2.793	2.718	-5.511	-2.164
FAYPIG	2.879	-2.876	2.818	-5.694	-2.815	4.551	-3.836	2.837	-6.673	-2.122
HUQGOR	1.174	-1.857	2.770	-4.627	-3.453	2.659	-2.665	2.771	-5.436	-2.777
HUQHAE	1.371	-1.796	2.713	-4.508	-3.137	2.897	-2.611	2.721	-5.332	-2.435
JENROM	1.519	-1.882	2.693	-4.574	-3.055	3.099	-2.695	2.700	-5.395	-2.296
OLEYAH	1.950	-1.529	3.899	-5.428	-3.478	3.634	-2.558	3.921	-6.478	-2.845
PUGSER	3.237	-3.067	3.090	-6.157	-2.921	4.860	-3.976	3.107	-7.082	-2.223
PUGSIV	2.771	-3.014	3.092	-6.106	-3.335	4.421	-3.956	3.109	-7.066	-2.644
PUGSOB	2.167	-2.416	3.235	-5.651	-3.484	3.584	-3.240	3.252	-6.491	-2.907
PUGSUH	2.546	-2.910	3.122	-6.032	-3.486	4.146	-3.850	3.139	-6.989	-2.844
WONZUV	2.716	-3.182	1.989	-5.171	-2.455	4.887	-4.633	1.988	-6.621	-1.733
YEKHUU	2.630	-1.931	3.175	-5.106	-2.476	4.301	-2.894	3.192	-6.085	-1.784
KUYGOC	2.332	-2.051	2.613	-4.664	-2.332	3.840	-2.901	2.622	-5.523	-1.683
LUMDIG	2.818	-1.448	4.334	-5.782	-2.963	4.500	-2.385	4.356	-6.741	-2.241
TULLIX	3.149	-2.103	3.999	-6.102	-2.953	4.689	-2.963	4.019	-6.982	-2.293
WORTAA	1.881	-1.384	3.734	-5.119	-3.238	3.220	-2.196	3.735	-5.931	-2.712
WUZGAB	2.474	-1.834	3.012	-4.846	-2.372	4.563	-3.183	3.015	-6.198	-1.635
YEKJEG	2.483	-2.457	2.950	-5.407	-2.924	4.134	-3.409	2.978	-6.387	-2.253

Table S9. Electronic band gap, fermi energy (given as the highest occupied level), electrostatic potential, IP and EA (all in eV) of 20 selected **DS2** computed at PBE level and corrected values by means of applying a systematic shift of -0.7 eV and +0.9 eV to the PBE IP and EA values.

	PBE					PBE-corrected		
	gap	fermi	work	IP	EA	gap	IP-0.7	EA+0.9
ASINAT	1.558	-1.713	2.891	-4.604	-3.046	3.158	-5.304	-2.146
ATAHUA	2.444	-0.429	4.911	-5.341	-2.897	4.044	-6.041	-1.997
BEDMOO	2.290	-1.720	4.219	-5.940	-3.650	3.890	-6.640	-2.750
CABJEX	3.085	-2.419	3.955	-6.374	-3.289	4.685	-7.074	-2.389
CAVRAU	3.240	-2.372	3.314	-5.685	-2.446	4.840	-6.385	-1.546
CAVREY	3.207	-2.267	3.594	-5.861	-2.654	4.807	-6.561	-1.754
CUBBEI	1.768	-2.427	2.452	-4.878	-3.110	3.368	-5.578	-2.210
DEVWOT	1.489	-1.315	4.244	-5.559	-4.070	3.089	-6.259	-3.170
ECOWUQ	1.996	-2.084	2.707	-4.791	-2.795	3.596	-5.491	-1.895
EMITOK	2.544	-1.916	4.333	-6.249	-3.706	4.144	-6.949	-2.806
EWOVET	1.906	-2.711	2.772	-5.483	-3.577	3.506	-6.183	-2.677
FANPAO	2.173	-2.184	4.316	-6.500	-4.328	3.773	-7.200	-3.428
FAYPIG	2.879	-2.876	2.818	-5.694	-2.815	4.479	-6.394	-1.915
FEHCOM	3.054	-2.177	3.368	-5.545	-2.490	4.654	-6.245	-1.590
GATJIV	2.092	-1.281	4.587	-5.869	-3.777	3.692	-6.569	-2.877
GEXPAD	2.677	-0.824	5.096	-5.920	-3.243	4.277	-6.620	-2.343
GUKPEJ	3.113	-0.080	5.638	-5.718	-2.605	4.713	-6.418	-1.705
GULWOA	3.090	-1.853	5.276	-7.128	-4.038	4.690	-7.828	-3.138
GUPBOJ	4.010	-0.424	4.566	-4.990	-0.980	5.610	-5.690	-0.080
HAJKIO	2.642	-1.093	3.704	-4.797	-2.155	4.242	-5.497	-1.255
HUQGOR	1.174	-1.857	2.770	-4.627	-3.453	2.774	-5.327	-2.553
HUQHAE	1.371	-1.796	2.713	-4.508	-3.137	2.971	-5.208	-2.237
HURFUX	2.599	-1.580	3.701	-5.281	-2.682	4.199	-5.981	-1.782
HUZFOY	2.856	-1.734	5.853	-7.587	-4.732	4.456	-8.287	-3.832
IQOJEF	2.028	-0.592	4.636	-5.228	-3.200	3.628	-5.928	-2.300
JABGUR	3.993	-1.109	4.482	-5.591	-1.598	5.593	-6.291	-0.698
JENROM	1.519	-1.882	2.693	-4.574	-3.055	3.119	-5.274	-2.155
KUYGOC	2.332	-2.051	2.613	-4.664	-2.332	3.932	-5.364	-1.432
LUMDEC	2.818	-1.451	3.672	-5.123	-2.305	4.418	-5.823	-1.405
LUMDIG	2.818	-1.448	4.334	-5.782	-2.963	4.418	-6.482	-2.063
MUQSAU	1.688	-1.017	4.540	-5.557	-3.868	3.288	-6.257	-2.968
NATHUO	3.017	-1.863	4.269	-6.132	-3.115	4.617	-6.832	-2.215
OFEHAK	3.084	-1.646	5.372	-7.018	-3.934	4.684	-7.718	-3.034
OFEHEO	2.416	-0.728	3.712	-4.441	-2.024	4.016	-5.141	-1.124
OHAPAQ	2.736	-0.877	3.945	-4.822	-2.086	4.336	-5.522	-1.186
OLEYAH	1.950	-1.529	3.899	-5.428	-3.478	3.550	-6.128	-2.578

OPOBIF	3.687	-0.304	5.891	-6.195	-2.508	5.287	-6.895	-1.608
PEKTUW	2.313	-1.814	3.669	-5.483	-3.170	3.913	-6.183	-2.270
PEMRIK	2.322	-1.558	4.265	-5.823	-3.501	3.922	-6.523	-2.601
PEQKUT	2.730	0.313	4.385	-4.072	-1.342	4.330	-4.772	-0.442
PUGSER	3.237	-3.067	3.090	-6.157	-2.921	4.837	-6.857	-2.021
PUGSIV	2.771	-3.014	3.092	-6.106	-3.335	4.371	-6.806	-2.435
PUGSOB	2.167	-2.416	3.235	-5.651	-3.484	3.767	-6.351	-2.584
PUGSUH	2.546	-2.910	3.122	-6.032	-3.486	4.146	-6.732	-2.586
PUSXIL	2.998	-2.565	4.296	-6.861	-3.863	4.598	-7.561	-2.963
QAFJEP	2.839	-0.444	5.280	-5.724	-2.885	4.439	-6.424	-1.985
QOJBAU	2.658	-1.946	4.145	-6.092	-3.433	4.258	-6.792	-2.533
RUCSEP	1.923	-0.961	4.575	-5.537	-3.614	3.523	-6.237	-2.714
RUGXIC	2.423	-2.089	3.289	-5.378	-2.954	4.023	-6.078	-2.054
SAKSOO	3.062	-1.034	5.777	-6.810	-3.749	4.662	-7.510	-2.849
SARNOQ	3.987	-3.178	3.506	-6.684	-2.697	5.587	-7.384	-1.797
SERWAP	2.705	-1.570	3.729	-5.298	-2.593	4.305	-5.998	-1.693
TELDOF	3.120	-0.220	2.964	-3.184	-0.064	4.720	-3.884	0.836
TUKDEK	2.685	-1.503	5.083	-6.585	-3.900	4.285	-7.285	-3.000
TULLIX	3.149	-2.103	3.999	-6.102	-2.953	4.749	-6.802	-2.053
VEXQIA	3.842	0.698	4.685	-3.988	-0.146	5.442	-4.688	0.754
VULWEF	1.760	-1.244	4.811	-6.055	-4.295	3.360	-6.755	-3.395
WARFAZ	1.605	-1.027	4.064	-5.091	-3.486	3.205	-5.791	-2.586
WEDSIK	3.037	-1.051	4.694	-5.745	-2.708	4.637	-6.445	-1.808
WITWIH	2.473	-1.640	4.490	-6.129	-3.656	4.073	-6.829	-2.756
WOMCUY	2.549	-0.654	4.592	-5.246	-2.697	4.149	-5.946	-1.797
WONZUV	2.716	-3.182	1.989	-5.171	-2.455	4.316	-5.871	-1.555
WORTAA	1.881	-1.384	3.734	-5.119	-3.238	3.481	-5.819	-2.338
WUZGAB	2.474	-1.834	3.012	-4.846	-2.372	4.074	-5.546	-1.472
XEJJII	1.707	-2.260	2.700	-4.959	-3.253	3.307	-5.659	-2.353
XEZNEY	3.049	-1.885	3.982	-5.867	-2.818	4.649	-6.567	-1.918
XOVZEO	2.883	-2.553	3.085	-5.638	-2.755	4.483	-6.338	-1.855
XUTMAC	2.142	0.519	4.058	-3.539	-1.397	3.742	-4.239	-0.497
XUVQOW	2.716	-0.824	4.910	-5.733	-3.017	4.316	-6.433	-2.117
YEKHUU	2.630	-1.931	3.175	-5.106	-2.476	4.230	-5.806	-1.576
YEKJEG	2.483	-2.457	2.950	-5.407	-2.924	4.083	-6.107	-2.024
ZEHJEE	2.650	-0.850	3.127	-3.977	-1.327	4.250	-4.677	-0.427
ZUCGAH	1.658	0.365	4.492	-4.127	-2.468	3.258	-4.827	-1.568