Supporting information for: Transferable forcefield for metal-organic frameworks from first-principles: BTW-FF

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Table S1: Structural properties of MOF-5, IRMOF-10 and IRMOF-14. All lattice parameters are reported as space group symmetry is not enforced.

	MOF-5			IRMOF-10			IRMOF-14		
	DFT	BTW-FF	Error (%)	DFT	BTW-FF	Error (%)	DFT	BTW-FF	Error (%)
Bond lengths (Å)									
913 - 902	1.489	1.494	0.34	1.478	1.494	1.07	1.489	1.494	0.33
902 - 912	1.400	1.403	0.21	1.400	1.404	0.28	1.397	1.404	0.50
903 - 912	-	-	-	1.410	1.402	0.57	-	-	-
903 - 903	-	-	-	1.475	1.497	1.47	-	-	-
912 - 912	1.389	1.398	0.65	1.387	1.399	0.86	1.399	1.403	0.29
913 - 170	1.273	1.269	0.31	1.277	1.270	0.55	1.274	1.271	0.24
Zn - 170	1.941	1.921	1.24	1.929	1.917	0.63	1.942	1.917	1.30
Zn - 171	1.943	1.911	1.65	1.934	1.911	1.74	1.942	1.911	1.62
Bond angles (°)									
170 - 913 - 170	126.2	126.9	0.55	126.4	126.8	0.33	126.1	126.7	0.49
Zn - 171 - Zn	109.5	109.5	0.00	109.5	109.5	0.00	109.5	109.5	0.00
171 - Zn - 170	111.8	112.4	0.51	112.1	112.5	0.29	111.9	112.5	0.58
913 - 170 - Zn	130.3	129.4	0.73	129.8	129.4	0.33	130.4	129.5	0.68
Parameters									
a (Å)	18.000	18.315	0.63	24.314	24.498	0.75	24.300	24.287	0.05
b (Å)	18.200	18.315	0.63	24.314	24.498	0.75	24.300	24.287	0.05
c (Å)	18.200	18.315	0.63	24.314	24.498	0.75	24.300	24.287	0.05
$\alpha(^\circ)$	60.0	60.0	0.00	60.0	60.0	0.00	60.0	60.0	0.00
$\beta(^\circ)$	60.0	60.0	0.00	60.0	60.0	0.00	60.0	60.0	0.00
$\gamma(^\circ)$	60.0	60.0	0.00	60.0	60.0	0.00	60.0	60.0	0.00

Table S2: Structural properties of UiO-66 and UiO-67. All lattice parameters are reported as space group symmetry is not enforced.

	UiO-66			UiO-67		
	DFT	BTW-FF	Error (%)	DFT	BTW-FF	Error (%)
Bond lengths (Å)						
913 - 902	1.492	1.497	0.34	1.496	1.497	0.07
902 - 912	1.400	1.403	0.21	1.401	1.405	0.29
912 -91 2	1.388	1.397	0.65	1.391	1.398	0.50
913 - 170	1.275	1.251	1.88	1.273	1.251	1.73
Zr - 170	2.218	2.234	0.72	2.252	2.234	0.80
Zr - 171	2.062	2.045	0.82	2.089	2.045	2.11
Zr - 75	2.256	2.204	2.23	2.285	2.224	2.67
Bond angles (°)						
170 - 913 - 170	125.3	126.6	1.02	125.3	126.6	1.07
Zr - 171 - Zr	117.1	119.0	1.64	117.4	117.7	0.55
171 - Zr - 170	83.3	85.8	3.00	84.2	85.4	1.43
913 - 170 - Zr	133.7	133.4	0.23	134.7	133.5	0.16
Parameters						
a (Å)	20.798	20.903	0.51	27.094	27.049	0.17
b (Å)	20.798	20.903	0.51	27.094	27.049	0.17
c (Å)	20.798	20.903	0.51	27.094	27.049	0.17
$\alpha(^\circ)$	90.0	90.0	0.00	90.0	90.0	0.00
$\beta(^\circ)$	90.0	90.0	0.00	90.0	90.0	0.00
$\gamma(^\circ)$	90.0	90.0	0.00	90.0	90.0	0.00

Table S3: Structural properties of HKUST-1. All lattice parameters are reported as space group symmetry is not enforced.

	HKUST-1		
	DFT	BTW-FF	Error (%)
Bond lengths (Å)			
913 - 902	1.491	1.496	0.34
902 - 912	1.396	1.404	0.57
913 - 170	1.275	1.287	0.94
Cu - 170	1.939	1.912	1.39
Cu - Cu	2.422	2.476	2.23
Bond angles (°)			
170 - 913 - 170	126.3	127.4	0.84
913 - 170 - Cu	118.9	118.7	0.19
Parameters			
a (Å)	26.300	26.290	0.04
b (Å)	26.300	26.290	0.04
c (Å)	26.300	26.290	0.04
$\alpha(^\circ)$	90.0	90.0	0.00
$\beta(^\circ)$	90.0	90.0	0.00
$\gamma(^\circ)$	90.0	90.0	0.00

Table S4: vdW radii and epsilon parameters for MOF-5, IRMOF-10 and IRMOF-14.

Atom type	Element	radii (Å)	ϵ (kcalmol^{-1})
912	C	1.9600	0.0560
913	C	1.9400	0.0560
915	H	1.6200	0.0200
170	O	1.8200	0.0590
171	O	1.820	0.0590
172	Zn	2.290	0.2760
902	C	1.9600	0.0560

Table S5: Bond stretch parameters for MOF-5, IRMOF-10 and IRMOF-14. Given are the force constants (k) and equilibrium bond lengths (r).

Bond	k (kcalmol^{-1} / Å^2)	r (Å)
912 - 915	5.150	1.1010
913 - 170	5.999	1.2990
913 - 902	5.299	1.4850
912 - 912	4.500	1.3890
902 - 912	4.500	1.3890
903 - 903	5.899	1.4650
903 - 912	5.999	1.3890
172 - 171	4.329	2.0390
172 - 170	3.665	2.0090

Table S6: Bond bending parameters for MOF-5, IRMOF-10 and IRMOF-14. Given are the force constants (k) and equilibrium bond angles (θ).

Bond	k (kcalmol^{-1} / radian^2)	θ (°)
170 - 913 - 170	2.867	126.299
902 - 913 - 170	1.867	117.082
171 - 172 - 170	3.000	113.584
172 - 170 - 913	3.022	130.606
170 - 172 - 170	1.000	110.103
172 - 171 - 172	1.198	110.992
912 - 902 - 912	0.000	119.406
902 - 912 - 912	0.060	121.582
912 - 902 - 913	0.360	121.797
902 - 912 - 915	0.090	119.859
912 - 903 - 912	5.000	117.621
903 - 912 - 912	5.000	122.904
903 - 912 - 915	5.000	120.000
903 - 903 - 912	5.000	122.690

Table S7: Out of plane bending parameters for MOF-5, IRMOF-10 and IRMOF-14. Given are the force constants (k).

Bond	k (kcalmol^{-1} / radian^2)
170 - 913 - 170 - 902	1.50
902 - 913 - 170 - 170	0.00
902 - 912 - 912 - 915	0.00
903 - 912 - 912 - 915	0.00

Table S8: Torsion parameters for MOF-5, IRMOF-10 and IRMOF-14. Given are the force constants (k), equilibrium phase angles (Φ_0) and integer periodicity (n).

Bond	k (kcalmol^{-1} / radian^2)	Φ_0	n
170 - 913 - 902 - 912	2.500	180.0	2
171 - 172 - 170 - 913	4.690	180.0	2
172 - 170 - 913 - 170	2.176	180.0	2
915 - 912 - 902 - 913	1.999	180.0	2
170 - 172 - 170 - 913	0.860	180.0	2
172 - 170 - 913 - 902	0.072	180.0	2
170 - 172 - 171 - 172	1.000	180.0	2
913 - 902 - 912 - 912	8.030	180.0	2
912 - 902 - 912 - 912	8.030	180.0	2
912 - 902 - 912 - 915	8.030	180.0	2
902 - 912 - 912 - 915	8.030	180.0	2
902 - 912 - 912 - 902	8.030	180.0	2
902 - 912 - 912 - 912	8.030	180.0	2
903 - 903 - 912 - 915	6.999	180.0	2
903 - 903 - 912 - 912	6.900	180.0	2
912 - 903 - 903 - 912	6.900	180.0	2
903 - 903 - 912 - 912	6.900	180.0	2
912 - 903 - 903 - 912	6.900	180.0	2
912 - 903 - 912 - 912	4.930	180.0	2
912 - 903 - 912 - 915	4.930	180.0	2
915 - 912 - 912 - 903	4.930	180.0	2
902 - 912 - 912 - 903	5.930	180.0	2
912 - 903 - 903 - 912	5.000	180.0	2

Table S9: vdW and epsilon parameters for UiO-66 and UiO-67.

Atom type	Element	vdW radii (Å)	ϵ (kcalmol^{-1})
912	C	1.96	0.056
913	C	1.94	0.056
915	H	1.62	0.020
21	H	1.60	0.020
170	O	1.82	0.059
171	O	1.82	0.059
192	Zr	3.52	0.367
902	C	1.96	0.056
75	O	1.82	0.059
903	C	1.96	0.056

Table S10: Bond stretch parameters for UiO-66 and UiO-67. Given are the force constants (k) and equilibrium bond lengths (r). Shown in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k (kcalmol^{-1} / Å^2)	r (Å)
912 - 915	5.150	1.1010
913 - 170	5.999	1.2990
913 - 902	5.229	1.4850
912 - 912	4.500	1.3890
912 - 902	4.500	1.3890
903 - 903	5.899	1.4650
903 - 912	5.999	1.3890
21 - 75	3.630	0.9890
192 - 171	5.809	2.1920
192 - 170	5.821	2.3380
75 - 192 (4)	5.500	2.2760
171 - 192 (4)	5.809	2.1920
75 - 192	5.500	2.2760

Table S11: Bond bending parameters for UiO-66 and UiO-67. Given are the force constants (k) and equilibrium bond angles (θ). Shown in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k (kcalmol^{-1} / radian^2)	θ (°)
170 - 913 - 170	2.867	126.299
902 - 913 - 170	1.867	117.082
912 - 902 - 912	0.000	119.406
902 - 912 - 912	0.060	121.582
912 - 902 - 913	0.360	121.797
902 - 912 - 915	0.090	118.859
903 - 903 - 912	5.000	122.690
912 - 903 - 912	5.000	117.621
903 - 912 - 912	5.000	122.904
903 - 912 - 915	5.000	120.000
171 - 192 - 170	2.099	84.318
192 - 170 - 913	2.099	139.820
170 - 192 - 170	2.099	73.103
192 - 171 - 192	2.099	118.053
21 - 75 - 192	2.099	116.848
192 - 75 - 192	2.099	103.406
192 - 171 - 192 (4)	2.099	118.408
170 - 192 - 75	2.099	89.658
171 - 192 - 75	2.099	71.110
192 - 75 - 192 (4)	2.099	103.406
75 - 192 - 75	2.099	123.230
75 - 192 - 171 (4)	2.099	71.110
171 - 192 - 171	2.099	91.479

Table S12: Out of plane bending parameters for UiO-66 and UiO-67. Given are the force constants (k).

Bond	k (kcalmol^{-1} / radian^2)
902 - 912 - 915 - 912	1.5
170 - 913 - 902 - 170	0.0
902 - 913 - 170 - 170	0.0
192 - 171 - 192 - 170	2.0

Table S13: Torsion parameters for UiO-66 and UiO-67. Given are the force constants (k), equilibrium phase angles (Φ_0) and integer periodicity (n). Shown in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k (kcalmol^{-1} / radian^2)	Φ_0	n
170 - 913 - 902 - 912	2.500	180.0	2
171 - 192 - 170 - 913	2.064	180.0	2
192 - 170 - 913 - 170	2.017	180.0	2
915 - 912 - 902 - 913	1.999	180.0	2
170 - 192 - 170 - 913	0.860	180.0	2
192 - 170 - 913 - 902	0.072	180.0	2
170 - 192 - 171 - 192	1.000	180.0	2
913 - 170 - 192 - 75	5.000	180.0	2
21 - 75 - 192 - 170	5.000	180.0	2
21 - 75 - 191 - 170	5.000	180.0	2
192 - 75 - 192 - 170	5.000	180.0	2
192 - 75 - 192 - 75	5.000	180.0	2
192 - 75 - 192 - 171	5.000	180.0	2
21 - 75 - 192 - 75	5.000	180.0	2
192 - 75 - 192 - 171 (4)	5.000	180.0	2
192 - 171 - 192 - 75	5.000	180.0	2
192 - 171 - 192 - 171	5.000	180.0	2
21 - 75 - 192 - 171	5.000	180.0	2
192 - 75 - 192 - 171 (4)	5.000	180.0	2
192 - 171 - 192 - 75 (4)	5.000	180.0	2
913 - 902 - 912 - 912	8.030	180.0	2
912 - 902 - 912 - 912	8.030	180.0	2
912 - 902 - 912 - 915	8.030	180.0	2
902 - 912 - 912 - 915	8.030	180.0	2
902 - 912 - 912 - 902	8.030	180.0	2
903 - 903 - 912 - 915	6.999	180.0	2
903 - 903 - 912 - 912	6.900	180.0	2
912 - 903 - 903 - 912	6.900	180.0	2
912 - 903 - 912 - 912	4.930	180.0	2
912 - 903 - 912 - 915	4.930	180.0	2
915 - 912 - 912 - 903	4.930	180.0	2
902 - 912 - 912 - 903	5.930	180.0	2
912 - 903 - 903 - 912	1.299	180.0	2

Table S14: vdW radii and epsilon parameters for HKUST-1.

Atom type	Element	vdW radii (Å)	ϵ (kcalmol^{-1})
912	C	1.96	0.056
913	C	1.94	0.056
915	H	1.62	0.020
170	O	1.82	0.059
902	C	1.96	0.056
185	Cu	2.29	0.276

Table S15: Bond stretch parameters for HKUST-1. Given are the force constants (k) and equilibrium bond lengths (r). Given in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k(kcalmol^{-1} / Å^2)	r (Å)
912 - 915	5.150	1.101
913 - 902	5.299	1.485
902 - 912	4.500	1.389
913 - 170 (5)	5.999	1.299
170 - 185 (5)	5.091	1.969
185 - 185 (5)	4.349	2.422

Table S16: Bond bending parameters for HKUST-1. Given are the force constants (k) and equilibrium bond angles (θ). Shown in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k (kcalmol^{-1} / radian^2)	θ (°)
902 - 913 - 170	1.867	117.082
170 - 185 - 170	0.050	175.945
170 - 913 - 170 (5)	2.867	126.299
913 - 170 - 185 (5)	3.322	120.962
170 - 185 - 185 (5)	4.299	87.822
902 - 912 - 902	0.060	121.797
912 - 902 - 913	0.360	121.797
912 - 902 - 912	0.000	119.406
902 - 912 - 915	0.390	119.859

Table S17: Out of plane bending parameters for HKUST-1. Given are the force constants (k).

Bond	k (kcalmol^{-1} / radian^2)
902 - 912 - 915 - 912	1.5
170 - 913 - 902 - 170	0.0
902 - 913 - 170 - 170	0.0
192 - 171 - 192 - 170	2.0

Table S18: Torsion parameters for UiO-66 and UiO-67. Given are the force constants (k), equilibrium phase angles (Φ_0) and integer periodicity (n). Shown in brackets are additional ring parameters as defined in MM3. The number within the bracket refers to the number of atoms in the ring.

Bond	k (kcalmol^{-1} / radian^2)	Φ_0	n
170 - 913 - 902 - 912	2.5	180.0	2
915 - 912 - 902 - 913	1.999	180.0	2
170 - 185 - 170 - 913	0.860	180.0	2
185 - 170 - 913 - 902	0.072	180.0	2
170 - 913 - 170 - 185 (5)	5.805	180.0	2
91 3 - 170 - 185 - 185 (5)	0.850	180.0	2
170 - 185 - 185 - 170	2.071	180.0	2
170 - 185 - 185 - 170 (5)	2.071	180.0	2
912 - 902 - 912 - 915	8.030	180.0	2
902 - 912 - 902 - 912	8.030	180.0	2
902 - 912 - 902 - 913	8.030	180.0	2

Table S19: Calculated modal heat capacities (C_V) for MOF-5, IRMOF-10, IRMOF-14, UiO-66, UiO-67 and HKUST-1.

	C_V (JK^{-1}mol^{-1})					
Temperature (K)	MOF-5	IRMOF-10	IRMOF-14	UiO-66	UiO-67	HKUST-1
80	38.7	54.6	68.5	39.0	55.2	58.6
130	49.4	71.4	89.3	51.2	73.2	75.1
180	54.8	81.7	99.6	57.7	83.8	83.2
230	57.9	87.3	105.2	61.5	90.5	87.7
280	59.8	91.2	109.0	63.8	94.8	90.3
330	61.1	93.8	111.0	65.3	97.7	92.0
380	61.9	95.7	113.0	66.3	99.7	93.2
430	62.5	97.0	114.0	67.0	101.0	94.0
480	62.9	97.9	115.0	67.5	102.0	94.5
500	63.1	98.6	115.0	67.7	103.0	94.7