SUPPLEMENTARY MATERIAL

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Improved predictive tools for structural properties of metal–organic frameworks

Indrani Choudhuri and Donald G. Truhlar*

Department of Chemistry, Chemical Theory Center, and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, Minnesota 55455, USA

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Table S1: Computational details and other related information of the test set of MOFs

MOF[a]	Reference Code[b]	Metal Center of MOF	Oxidation State of Metal[c]	*k* points[d]	Magnetic State[e]	Initial Spin State of the Metal Ions Considered[f]	Temperatures (K) of X-ray Measurements	Reference[g]
$Ag_4C_{12}Cl_4O_8$	RORQOE	Ag	I	6×4×2	NM	--	293	1
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	GUPCUQ01	Cd	II	2×2×2	NM	--	293	2
$Cd_2H_{10}C_{16}N_4O_{10}$	PIJGEV	Cd	II	4×4×4	NM	--	295	3
$Zn_1H_4C_4O_4$	OFUWIV01	Zn	II	6×6×4	NM	--	293	4
$Li_8Zn_8H_{24}C_{72}O_{48}$	WAJJAU	Li, Zn	Li (I), Zn (II)	2×2×2	NM	--	293	5
$Co_2C_8N_{12}$	HAWVOQ01	Co	II	4×4×4	FM	3, 3	150	6
$Cu_3H_4C_{10}O_{10}$	MURCEH	Cu	II	4×4×2	AFM	–1, –1, 1, 1, –1, 1	293	7
$Cu_8H_8C_8N_{12}Cl_8$	QEJZUB01	Cu	I and II	4×4×2	AFM	1, –1, 1, –1,	90	8
$Dy_2H_{12}C_{12}N_2O_{16}$	YORSII	Dy	III	4×4×2	FM	5, 5	298	9
$Fe_4H_4C_4O_{12}$	HOGWAB	Fe	II	4×4×4	AFM	4, –4, 4, –4	283-303	10
$Fe_4P_4H_{16}C_8O_{24}$	DEMLIR	Fe	III	4×4×2	AFM	5, –5, 5, –5	298	11
$Sm_2H_{12}C_{10}O_{14}$	KOMJEC	Sm	III	4×4×4	AFM	5, –5	293	12
$Zr_{24}O_{128}C_{192}$ (UiO-66)	RUBTAK	Zr	IV	2×2×2	NM	--	298	13
$Zn_{32}O_{104}C_{192}H_{96}$ (MOF-5)	SAHYIK	Zn	II	2×2×2	NM	--	213	14

[a] Chemical formula of the unit cell

[b] The reference code associated with the structure in the Cambridge Structural Database (CSD) and CoRE MOF database.

[c] Oxidation states of the metal center according to the experimental reference

[d] *k*-points grid used for the calculations

[e] Magnetic ground state considered for the calculations

[f] Initial multiplicities of the metal ions considered for the calculations of the FM and AFM MOFs

[g] Experimental reference for the MOF

Table S2: Lattice constants (Å) of metal–organic frameworks (MOFs)

MOF	Exp.[a]	MN15–L	PBE	PBEsol	PBE–D2	PBE–D3	revM06–L	revTPSS	SCAN	SOGGA	vdW–DF2
$Ag_4C_{12}Cl_4O_8$	*a*=5.29	*a*=5.16	*a*=5.79	*a*=5.46	*a*=5.43	*a*=5.39	*a*=5.22	*a*=5.66	*a*=5.26	*a*=5.44	*a*=5.49
	b=6.34	*b*=6.52	*b*=6.06	*b*=6.10	*b*=6.38	*b*=6.34	*b*=6.39	*b*=5.99	*b*=6.29	*b*=6.08	*b*=6.48
	c=11.40	*c*=11.52	*c*=12.38	*c*=11.65	*c*=10.75	*c*=11.43	*c*=11.59	*c*=12.21	*c*=11.36	*c*=11.61	*c*=11.67
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	*a*=18.07	*a*=17.94	*a*=18.34	*a*=18.08	*a*=18.14	*a*=18.22	*a*=18.08	*a*=18.30	*a*=18.06	*a*=18.07	*a*=18.4
	b=18.07	*b*=17.94	*b*=18.34	*b*=18.08	*b*=18.14	*b*=18.22	*b*=18.08	*b*=18.30	*b*=18.06	*b*=18.07	*b*=18.4
	c=18.07	*c*=17.94	*c*=18.34	*c*=18.08	*c*=18.14	*c*=18.22	*c*=18.08	*c*=18.30	*c*=18.06	*c*=18.07	*c*=18.4
$Cd_2H_{10}C_{16}N_4O_{10}$	*a*=7.55	*a*=7.42	*a*=7.82	*a*=7.64	*a*=7.58	*a*=7.69	*a*=7.51	*a*=7.71	*a*=7.56	*a*=7.62	*a*=7.68
	b=7.64	*b*=7.49	*b*=7.84	*b*=7.74	*b*=7.66	*b*=7.77	*b*=7.57	*b*=7.76	*b*=7.67	*b*=7.74	*b*=7.78
	c=8.47	*c*=8.50	*c*=8.63	*c*=8.42	*c*=8.54	*c*=8.50	*c*=8.45	*c*=8.58	*c*=8.39	*c*=8.41	*c*=8.65
$Zn_1H_4C_4O_4$	*a*=4.83	*a*=4.83	*a*=4.96	*a*=4.87	*a*=4.87	*a*=4.90	*a*=4.74	*a*=4.94	*a*=4.83	*a*=4.87	*a*=4.90
	b=4.83	*b*=4.83	*b*=4.96	*b*=4.87	*b*=4.87	*b*=4.90	*b*=4.74	*b*=4.94	*b*=4.83	*b*=4.87	*b*=4.90
	c=6.25	*c*=6.54	*c*=6.46	*c*=6.30	*c*=6.20	*c*=6.35	*c*=6.38	*c*=6.41	*c*=6.25	*c*=6.30	*c*=6.37
$Li_8Zn_8H_{24}C_{72}O_{48}$	*a*=16.34	*a*=16.49	*a*=16.51	*a*=16.36	*a*=16.47	*a*=16.47	*a*=16.35	*a*=16.46	*a*=16.30	*a*=16.36	*a*=16.74
	b=16.34	*b*=16.49	*b*=16.51	*b*=16.36	*b*=16.47	*b*=16.47	*b*=16.35	*b*=16.46	*b*=16.30	*b*=16.36	*b*=16.74
	c=11.28	*c*=11.32	*c*=11.4	*c*=11.31	*c*=11.28	*c*=11.31	*c*=11.27	*c*=11.34	*c*=11.25	*c*=11.31	*c*=11.66
$Co_2C_8N_{12}$	*a*=5.97	*a*=5.11	*a*=6.17	*a*=5.89	*a*=5.83	*a*=5.87	*a*=5.95	*a*=5.95	*a*=5.87	*a*=6.37	*a*=5.86
	b=7.06	*b*=6.49	*b*=7.09	*b*=6.98	*b*=6.98	*b*=7.02	*b*=7.05	*b*=7.03	*b*=6.95	*b*=6.72	*b*=6.97
	c=7.41	*c*=7.59	*c*=7.35	*c*=7.29	*c*=7.39	*c*=7.39	*c*=7.36	*c*=7.31	*c*=7.26	*c*=7.29	*c*=7.23
$Cu_3H_4C_{10}O_{10}$	*a*=10.03	*a*=10.10	*a*=10.29	*a*=10.01	*a*=10.03	*a*=9.98	*a*=10.00	*a*=10.12	*a*=9.97	*a*=10.02	*a*=10.08
	b=5.81	*b*=5.80	*b*=6.07	*b*=5.91	*b*=5.89	*b*=5.97	*b*=5.89	*b*=5.88	*b*=5.87	*b*=5.84	*b*=5.91
	c=9.63	*c*=9.74	*c*=9.68	*c*=9.61	*c*=9.66	*c*=9.68	*c*=9.58	*c*=9.65	*c*=9.56	*c*=9.59	*c*=9.75
$Cu_8H_8C_8N_{12}Cl_8$	*a*=6.77	*a*=6.79	*a*=6.99	*a*=6.81	*a*=6.74	*a*=6.85	*a*=6.79	*a*=6.84	*a*=6.81	*a*=6.89	*a*=6.98
	b=6.89	*b*=6.85	*b*=7.21	*b*=6.96	*b*=6.93	*b*=6.91	*b*=6.95	*b*=7.09	*b*=6.97	*b*=6.86	*b*=7.10
	c=12.36	*c*=12.42	*c*=12.29	*c*=12.16	*c*=12.29	*c*=12.29	*c*=12.16	*c*=12.40	*c*=12.19	*c*=12.19	*c*=12.2
$Dy_2H_{12}C_{12}N_2O_{16}$	*a*=6.74	*a*=6.55	*a*=6.83	*a*=6.68	*a*=6.66	*a*=6.72	*a*=6.77	*a*=6.82	*a*=6.70	*a*=6.69	*a*=6.78
	b=7.81	*b*=7.78	*b*=8.02	*b*=7.90	*b*=7.78	*b*=7.89	*b*=7.77	*b*=7.92	*b*=7.78	*b*=7.89	*b*=7.91
	c=9.17	*c*=9.33	*c*=9.29	*c*=9.17	*c*=9.19	*c*=9.26	*c*=9.16	*c*=9.24	*c*=9.15	*c*=9.18	*c*=9.33
$Fe_4H_4C_4O_{12}$	*a*=5.93	*a*=5.64	*a*=5.78	*a*=5.68	*a*=5.87	*a*=5.87	*a*=5.92	*a*=5.68	*a*=5.92	*a*=6.26	*a*=6.19
	b=5.54	*b*=5.17	*b*=5.31	*b*=5.30	*b*=5.63	*b*=5.47	*b*=5.53	*b*=5.44	*b*=5.75	*b*=5.83	*b*=5.78
	c=7.27	*c*=7.07	*c*=7.48	*c*=7.52	*c*=7.37	*c*=7.32	*c*=7.27	*c*=7.48	*c*=7.07	*c*=7.02	*c*=7.42
$Fe_4P_4H_{16}C_8O_{24}$	*a*=6.61	*a*=6.29	*a*=6.77	*a*=6.74	*a*=6.83	*a*=6.78	*a*=6.52	*a*=6.71	*a*=6.63	*a*=6.68	*a*=6.66
	b=8.36	*b*=8.23	*b*=8.46	*b*=8.30	*b*=8.21	*b*=8.54	*b*=8.36	*b*=8.46	*b*=8.30	*b*=8.30	*b*=8.44
	c=9.62	*c*=9.69	*c*=9.74	*c*=9.40	*c*=9.40	*c*=9.88	*c*=9.72	*c*=9.68	*c*=9.57	*c*=9.59	*c*=9.76
$Sm_2H_{12}C_{10}O_{14}$	*a*=6.76	*a*=6.91	*a*=6.75	*a*=6.65	*a*=6.69	*a*=6.67	*a*=6.83	*a*=6.74	*a*=6.72	*a*=6.65	*a*=6.85
	b=7.67	*b*=7.20	*b*=8.02	*b*=7.77	*b*=7.58	*b*=7.73	*b*=7.35	*b*=7.91	*b*=7.53	*b*=7.77	*b*=7.58
	c=8.05	*c*=7.89	*c*=8.19	*c*=8.04	*c*=7.90	*c*=8.12	*c*=7.99	*c*=8.19	*c*=8.00	*c*=8.03	*c*=8.19
UiO-66	*a=b=c=* 20.70	*a=b=c=* 20.61	*a=b=c=* 21.12	*a=b=c=* 20.96	*a=b=c=* 21.08	*a=b=c=* 21.07	*a=b=c=* 20.57	*a=b=c=* 21.11	*a=b=c=* 20.63	*a=b=c=* 20.95	*a=b=c=* 20.16
MOF-5	*a=b=c=* 25.66	*a=b=c=* 25.86	*a=b=c=* 26.09	*a=b=c=* 25.88	*a=b=c=* 25.07	*a=b=c=* 26.06	*a=b=c=* 25.79	*a=b=c=* 26.01	*a=b=c=* 25.83	*a=b=c=* 25.86	*a=b=c=* 26.19
MSE		**-0.05**	**0.20**	**-0.03**	**0.04**	**0.09**	**-0.02**	**0.13**	**-0.02**	**0.04**	**0.19**
MUE		**0.16**	**0.26**	**0.11**	**0.15**	**0.14**	**0.07**	**0.18**	**0.06**	**0.12**	**0.22**
MUPA (%)		**2.09**	**2.81**	**1.26**	**1.39**	**1.34**	**0.78**	**1.83**	**0.72**	**1.42**	**2.04**

[a] The references for the experimental lattice constants are given in table S1.

Table S3: Unit cell volumes (Å^3) of the metal–organic frameworks (MOFs)

MOF	Exp.[a]	MN15-L	PBE	PBEsol	PBE–D2	PBE–D3	revM06 –L	revTPSS	SCAN	SOGGA	vdW –DF2
$Ag_4C_{12}Cl_4O_8$	382.09	387.73	427.34	386.54	372.05	390.65	386.54	409.06	375.79	383.00	415.59
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	5907.36	5771.61	6167.81	5914.82	5968.28	6045.56	5910.69	6127.55	5892.93	5900.64	6232.68
$Cd_2H_{10}C_{16}N_4O_{10}$	435.56	431.81	464.86	437.40	434.76	445.74	431.93	453.66	430.46	435.95	457.62
$Zn_1H_4C_4O_4$	134.58	119.55	147.97	137.48	135.19	141.69	126.46	142.13	134.29	137.34	138.13
$Li_8Zn_8H_{24}C_{72}O_{48}$	3011.16	3080.00	3107.53	3027.04	3057.86	3067.34	3012.63	3072.81	2988.82	3027.40	3272.48
$Co_2C_8N_{12}$	312.15	532.18	334.29	299.48	284.90	288.37	308.76	305.49	296.18	312.15	295.51
$Cu_3H_4C_{10}O_{10}$	552.22	560.24	592.33	559.34	575.42	567.42	540.48	565.84	549.60	562.22	582.48
$Cu_8H_8C_8N_{12}Cl_8$	576.57	578.06	619.38	575.69	573.49	582.02	573.95	601.84	579.22	570.57	604.48
$Dy_2H_{12}C_{12}N_2O_{16}$	448.06	423.43	477.26	451.41	433.57	450.79	442.18	465.79	439.80	452.50	459.15
$Fe_4H_4C_4O_{12}$	238.62	206.60	229.25	224.78	243.18	235.19	238.69	231.17	238.62	245.38	266.13
$Fe_4P_4H_{16}C_8O_{24}$	531.61	502.13	558.15	526.17	527.66	572.86	529.45	549.75	526.61	539.61	548.27
$Sm_2H_{12}C_{10}O_{14}$	384.47	364.78	409.14	382.35	367.92	388.02	370.66	400.90	373.01	356.55	394.03
UiO-66	8870.26	8756.44	9429.46	9218.97	9371.18	9353.97	8714.89	9408.56	8802.82	9200.85	9407.48
MOF-5	16913.2	17311.9	17769.4	17337	17717.2	17703.6	17171.7	17603.01	17249.9	17294.9	17602
MSE		-19.69	145.44	55.75	-97.48	109.66	-1.67	-34.30	12.86	51.08	-173.85
MUE		33.69	146.78	6.50	108.36	113.55	8.22	36.65	35.61	56.89	173.85
MUPE (%)		**5.71**	**6.62**	**1.74**	**2.85**	**3.33**	**1.59**	**3.86**	**1.32**	**1.73**	**5.43**

[a] The experimental unit cell volume is calculated using the zeo++ software.[15,16,17]

Table S4: Pore diameters (Å) of the metal–organic frameworks (MOFs)

MOF	Acc.[a]		MN15-L		PBE		PBEsol		PBE–D2		PBE–D3		revM06-L		revTPSS		SCAN		SOGGA		vdW-DF2	
	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD	LCD	PLD
$Ag_4C_{12}Cl_4O_8$	1.36	1.30	1.48	1.47	1.65	1.65	1.47	1.47	1.32	1.32	1.37	1.31	1.32	1.26	1.53	1.53	1.32	1.32	1.45	1.45	1.48	1.35
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	12.58	12.58	12.43	12.43	12.72	12.72	12.49	12.49	12.53	12.53	12.60	12.60	12.57	12.57	12.70	12.70	12.45	12.45	12.48	12.48	12.72	12.72
$Cd_2H_{10}C_{16}N_4O_{10}$	2.02	2.02	1.97	1.95	2.07	2.06	2.03	2.03	1.99	1.97	2.05	2.02	2.01	2.01	2.09	2.09	2.01	2.01	2.02	2.02	2.13	2.13
$Zn_1H_4C_4O_4$	1.70	1.70	1.74	1.74	1.85	1.85	1.73	1.73	1.63	1.63	1.72	1.72	1.61	1.61	1.82	1.82	1.63	1.63	1.73	1.73	1.51	1.51
$Li_8Zn_8H_{24}C_{72}O_{48}$	7.48	7.48	7.5	7.5	7.52	7.52	7.43	7.43	7.50	7.49	7.50	7.49	7.43	7.43	7.47	7.47	7.39	7.39	7.43	7.43	7.66	7.66
$Co_2C_8N_{12}$	1.85	1.85	1.71	1.71	2.02	2.02	1.80	1.80	1.67	1.67	1.63	1.57	1.84	1.84	1.82	1.82	1.77	1.77	1.80	1.80	1.80	1.67
$Cu_3H_4C_{10}O_{10}$	1.80	1.80	1.7	1.7	1.93	1.93	1.70	1.62	1.75	1.75	1.72	1.72	1.65	1.65	1.76	1.76	1.70	1.70	1.70	1.70	1.77	1.70
$Cu_8H_8C_8N_{12}Cl_8$	1.37	1.29	1.35	1.26	1.53	1.51	1.41	1.37	1.38	1.18	1.43	1.29	1.39	1.33	1.48	1.45	1.42	1.34	1.41	1.34	1.49	1.27
$Dy_2H_{12}C_{12}N_2O_{16}$	1.81	1.81	1.66	1.65	1.82	1.77	1.69	1.69	1.54	1.54	1.56	1.66	1.75	1.70	1.79	1.79	1.65	1.63	1.71	1.71	1.65	1.65
$Fe_4H_4C_4O_{12}$	1.21	1.21	1.05	1.02	1.07	1.01	1.08	1.05	1.07	1.03	1.20	1.54	1.13	1.11	1.23	1.20	1.23	1.23	1.41	1.40	1.37	1.36
$Fe_4P_4H_{16}C_8O_{24}$	1.37	1.35	1.24	1.24	1.46	1.36	1.39	1.38	1.37	1.25	1.49	1.55	1.31	1.29	1.44	1.31	1.37	1.23	1.35	1.28	1.41	1.27
$Sm_2H_{12}C_{10}O_{14}$	1.36	1.30	1.5	1.74	1.93	1.91	1.92	1.92	1.86	1.50	1.96	1.90	1.81	1.78	1.95	1.95	1.92	1.92	1.92	1.90	1.99	1.99
UiO-66	8.88	3.79	8.82	3.76	9.37	4.05	9.26	3.99	9.34	4.03	9.09	3.92	8.80	3.74	9.12	3.93	8.75	3.71	9.26	3.98	9.39	4.06
MOF-5	14.94	7.84	15.08	7.92	15.24	8.03	15.10	7.93	15.23	8.02	15.23	8.02	15.03	7.89	15.18	7.99	15.06	7.92	15.08	7.92	15.32	8.08
MSE			-0.07	-0.06	0.13	0.10	0.02	-0.001	-0.01	-0.07	-0.01	0.03	-0.05	-0.05	0.07	0.06	-0.04	-0.04	0.03	0.02	0.10	0.04
MUE			**0.12**	**0.10**	**0.15**	**0.13**	**0.09**	**0.09**	**0.12**	**0.14**	**0.10**	**0.10**	**0.06**	**0.06**	**0.09**	**0.08**	**0.07**	**0.08**	**0.09**	**0.08**	**0.16**	**0.14**
MUPE (%)			**5.95**	**5.62**	**6.43**	**7.29**	**3.43**	**4.65**	**4.15**	**6.89**	**4.03**	**5.56**	**3.00**	**3.47**	**3.62**	**4.19**	**2.65**	**3.34**	**3.62**	**4.23**	**5.72**	**5.92**

[a] The accurate unit cell volume is calculated using the zeo++ software.[15,16,17]

Table S5: Bond lengths (Å) of the metal–organic frameworks (MOFs)

MOF	Bond length type	Exp.[a]	MN15–L	PBE	PBEsol	PBE–D2	PBE–D3	revM06–L	revTPSS	SCAN	SOGGA	vdW–DF2
$Ag_4C_{12}Cl_4O_8$	Ag-O	2.375	2.500	2.441	2.327	2.504	2.425	2.459	2.341	2.388	2.298	2.469
		2.468	2.522	2.38	2.41	2.451	2.474	2.496	2.502	2.471	2.444	2.527
		2.442	2.494	2.543	2.393	2.359	2.380	2.421	2.383	2.369	2.319	2.436
		2.461	2.519	2.565	2.453	2.452	2.457	2.462	2.407	2.408	2.386	2.469
	Ag-Cl	2.815	2.952	2.907	2.811	2.75	2.829	2.883	2.878	2.811	2.800	2.893
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	Cd-N	2.246	2.266	2.298	2.256	2.266	2.279	2.25	2.289	2.265	2.252	2.297
$Cd_2H_{10}C_{16}N_4O_{10}$	Cd-N	2.406	2.428	2.421	2.378	2.421	2.412	2.43	2.417	2.388	2.371	2.428
		2.511	2.573	2.56	2.49	2.56	2.543	2.541	2.521	2.504	2.479	2.548
	Cd-O	2.332	2.396	2.373	2.358	2.373	2.358	2.372	2.359	2.354	2.353	2.395
		2.321	2.328	2.395	2.356	2.395	2.376	2.324	2.363	2.333	2.352	2.37
		2.527	2.635	2.641	2.543	2.652	2.584	2.571	2.582	2.52	2.542	2.57
		2.299	2.403	2.332	2.285	2.332	2.31	2.355	2.335	2.305	2.281	2.355
		2.289	2.291	2.381	2.329	2.382	2.349	2.287	2.334	2.31	2.328	2.339
$Zn_1H_4C_4O_4$	Zn-O	1.943	1.984	1.981	1.952	1.973	1.974	1.937	1.977	1.944	1.95	1.981
		1.947	1.977	1.983	1.952	1.965	2.017	1.935	1.983	1.946	1.951	1.995
$Li_8Zn_8H_{24}C_{72}O_{48}$	Li-O	1.866	1.876	1.886	1.87	1.879	1.878	1.891	1.874	1.867	1.87	1.895
		2.001	2.02	2.03	1.993	1.999	2.02	2.07	2.001	1.988	1.993	2.048
		2.018	1.925	2.035	2.0152	2.088	2.039	2.076	2.016	1.995	2.015	2.053
		1.905	2.023	1.918	1.897	1.895	2.003	1.948	1.921	2.001	1.897	1.998
	Zn-O	1.900	1.936	1.932	1.907	1.926	1.926	1.922	1.936	1.901	1.907	1.943
$Co_2C_8N_{12}$	Co-N	2.096	2.013	2.048	2.017	1.940	1.909	2.084	2.030	2.011	1.992	1.909
		2.153	2.113	2.315	2.128	2.148	2.147	2.165	2.160	2.121	2.115	2.322
$Cu_3H_4C_{10}O_{10}$	Cu-O	1.951	1.982	1.99	1.938	1.965	1.969	1.945	1.949	1.928	1.923	1.981
		1.978	2.005	2.027	1.985	2.002	2.000	1.976	1.987	1.96	1.981	2.022
		1.956	1.989	2.05	1.974	1.983	1.985	1.966	1.954	1.942	1.951	2.011
		1.937	1.987	2.165	1.936	1.951	1.949	1.942	1.940	1.918	1.905	1.959
		2.103	2.089	2.141	2.096	2.127	2.154	2.124	2.110	2.094	2.0816	2.158
$Cu_8H_8C_8N_{12}Cl_8$	Cu-Cl	2.409	2.466	2.468	2.403	2.435	2.447	2.442	2.430	2.421	2.416	2.504
	Cu-N	1.937	1.964	2.165	1.919	1.941	1.943	1.925	1.960	1.924	1.918	1.987

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MOF	Bond length type	Exp.[a]	MN15–L	PBE	PBEsol	PBE–D2	PBE–D3	revM06–L	revTPSS	SCAN	SOGGA	vdW–DF2
$Dy_2H_{12}C_{12}N_2O_{16}$	Dy-O	2.377	2.357	2.385	2.359	2.359	2.374	2.352	2.366	2.344	2.341	2.456
		2.405	2.423	2.418	2.359	2.370	2.386	2.412	2.421	2.382	2.363	2.499
		2.289	2.281	2.308	2.274	2.278	2.305	2.287	2.298	2.275	2.272	2.313
		2.336	2.429	2.363	2.32	2.331	2.297	2.356	2.343	2.324	2.315	2.367
		2.266	2.208	2.349	2.275	2.258	2.278	2.233	2.287	2.256	2.275	2.28
		2.388	2.385	2.432	2.401	2.408	2.449	2.4	2.407	2.387	2.391	2.425
		2.423	2.411	2.506	2.476	2.542	2.506	2.437	2.465	2.457	2.478	2.491
		2.398	2.503	2.433	2.401	2.45	2.444	2.422	2.420	2.411	2.394	2.449
$Fe_4H_4C_4O_{12}$	Fe-O	2.060	1.987	2.113	2.118	2.097	2.121	2.018	2.099	1.996	2.006	2.129
		2.091	2.005	2.055	2.081	2.07	2.189	2.061	2.150	2.029	2.002	2.129
		2.157	2.027	2.09	2.042	2.057	2.033	2.169	2.077	2.209	2.25	2.234
		2.145	1.915	2.064	2.021	2.051	2.088	2.209	2.031	2.094	1.96	2.03
		2.194	2.211	2.288	2.248	2.328	2.218	2.247	2.160	2.264	2.25	2.138
		2.265	2.105	2.23	2.166	2.238	2.194	2.271	2.102	2.264	2.165	2.042
$Fe_4P_4H_{16}C_8O_{24}$	Fe-O	2.103	1.978	1.987	1.999	1.932	1.929	2.021	1.933	2.016	2.003	1.938
		1.941	1.938	1.968	1.945	1.961	1.96	1.938	1.965	1.94	1.93	1.987
		1.919	1.967	2.002	1.967	1.974	1.99	1.962	1.988	1.969	1.976	1.993
		2.008	1.985	2.04	2.068	2.066	2.096	2.011	2.026	2.009	2.000	2.098
		1.961	2.085	1.997	1.991	1.997	2.062	1.937	2.130	2.037	2.086	2.148
		2.103	2.089	2.141	2.096	2.127	2.154	2.124	2.110	2.094	2.0816	2.158
$Sm_2H_{12}C_{10}O_{14}$	Sm-O	2.402	2.384	2.294	2.28	2.474	2.294	2.356	2.294	2.306	2.278	2.3235
		2.423	2.411	2.513	2.398	2.372	2.409	2.426	2.417	2.412	2.394	2.49
		2.440	2.489	2.97	2.405	2.391	2.654	2.468	2.447	2.417	2.402	2.469
		2.403	2.534	2.138	2.378	2.29	2.406	2.465	2.398	2.407	2.373	2.445
		2.309	2.408	2.406	2.398	2.343	2.417	2.35	2.426	2.396	2.3987	2.422
		2.504	2.535	2.55	2.524	2.515	2.545	2.555	2.541	2.536	2.515	2.571
		2.549	2.494	2.589	2.489	2.546	2.52	2.4953	2.498	2.476	2.483	2.439
		2.456	2.458	2.501	2.472	2.372	2.478	2.462	2.474	2.455	2.469	2.474
UiO-66	Zr-O	2.23	2.22	**2.26**	**2.23**	**2.25**	**2.27**	2.22	2.27	2.22	2.22	2.26
		2.10	2.09	**2.13**	**2.12**	**2.13**	**2.14**	2.09	2.14	2.11	2.11	2.15
MOF-5	Zn-O	1.91	1.92	**1.97**	**1.94**	**1.96**	**1.96**	1.92	1.96	1.93	1.93	1.98
MSE (Å)			**0.014**	**0.04**	**-0.008**	**0.008**	**0.02**	**0.012**	**0.008**	**-0.005**	**-0.015**	**0.03**
MUE (Å)			**0.054**	**0.069**	**0.031**	**0.045**	**0.049**	**0.026**	**0.039**	**0.027**	**0.037**	**0.064**
MUPE (%)			**2.46**	**3.05**	**1.38**	**2.02**	**2.24**	**1.16**	**1.79**	**1.22**	**1.68**	**2.95**

[a] The references for the experimental bond lengths are given in Table S1.

Table S6: Bond angles (deg) of the metal–organic frameworks (MOFs) calculated using various functionals.

MOF	Bond angle type	Exp.[a]	MN15–L	PBE	PBEsol	PBE–D2	PBE–D3	revM06–L	revTPSS	SCAN	SOGGA	vdW–DF2
$Ag_4C_{12}Cl_4O_8$		65.96	64.73	65.57	66.82	66.46	65.93	64.91	66.14	66.21	67.02	64.4
	O-Ag-O	74.16	71.33	75.24	73.01	77.00	74.71	73.27	72.90	72.76	72.74	75.09
		108.82	110.25	110.64	117.90	98.41	110.53	112.51	122.49	112.35	117.94	110.85
		110.23	116.55	103.76	107.67	109.21	111.42	111.84	103.61	110.46	107.70	110.98
		137.82	132.08	135.44	134.00	131.55	136.66	164.62	122.49	135.33	133.91	137.05
		139.57	145.16	145.14	143.14	143.13	139.42	142.29	143.42	140.89	142.94	142.01
	O-Ag-Cl	74.94	78.09	74.32	72.69	77.63	75.29	75.57	73.16	73.58	72.60	75.63
		68.37	66.26	79.13	70.40	68.73	68.80	67.10	69.21	69.23	70.67	66.12
		137.90	139.41	132.12	133.66	142.81	139.5	136.15	131.89	136.31	133.73	134.76
		135.63	132.56	130.76	127.39	136.71	135.18	132.99	125.63	134.30	127.48	136.79
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	N-Cd-N	131.10	137.36	133.00	133.00	133.18	133.12	131.57	132.75	133.98	132.96	134
		99.85	97.59	99.14	99.14	99.08	99.10	99.68	99.23	98.78	99.16	98.78
$Cd_2H_{10}C_{16}N_4O_{10}$	N-Cd-N	66.38	65.96	66.19	67.55	66.19	66.63	65.52	66.43	66.81	67.77	66.46
	N-Cd-O	74.73	77.54	73.80	74.21	73.80	74.57	76.08	74.01	75.13	74.22	75.5
	N-Cd-O	82.18	83.29	83.79	82.01	75.06	82.47	82.35	82.60	81.91	82.00	81.68
		97.58	89.95	101.34	100.53	101.34	99.87	94.71	99.28	98.67	100.51	97.68
		75.99	75.13	75.06	75.41	75.06	75.62	75.86	75.72	75.95	75.44	75.82
	O-Cd-O	84.29	81.48	83.95	84.91	83.95	85.23	82.19	83.37	83.99	84.78	83.98
		85.42	86.93	83.20	83.32	83.20	84.34	86.35	83.27	84.10	83.15	85.17
		84.52	89.27	81.77	81.39	81.77	81.73	85.69	83.45	83.24	81.43	83.35
$Zn_1H_4C_4O_4$		102.9	105.55	101.07	101.85	102.87	103.11	105.18	100.70	101.70	101.82	105.54
	O-Zn-O	114.89	112.23	112.49	112.83	115.51	115.82	113.93	112.38	114.63	112.83	115.92
		107.1	107.01	107.33	106.45	109.49	108.76	108.53	107.08	109.38	106.44	107.33
$Li_8Zn_8H_{24}C_{72}O_{48}$		105.55	103.90	106.68	105.25	106.70	105.54	105.52	105.13	104.61	105.25	105.44
	O-Li-O	84.15	84.65	84.35	84.14	83.53	83.92	84.84	84.17	84.44	84.14	84.99
		137.90	139.14	137.12	137.66	136.41	138.40	138.21	135.83	137.97	137.66	138.64
		107.70	107.98	109.19	108.78	111.00	109.39	107.69	108.35	108.20	108.78	108.93
		94.12	93.25	93.29	93.30	94.76	93.89	93.34	91.91	93.18	93.30	95.58
	O-Zn-O	116.94	117.66	116.95	117.53	115.88	116.79	116.92	117.71	117.92	117.53	116.02
		121.28	121.28	121.29	121.10	121.47	121.29	122.07	120.90	121.00	121.10	122.42
	Li-O-Zn	94.09	93.87	93.91	94.31	95.10	94.52	93.67	94.52	93.86	94.31	94.35
		95.20	95.80	95.52	95.43	93.99	95.58	95.32	96.03	95.52	95.43	96.59

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MOF	Bond angle type	Exp.[a]	MN15−L	PBE	PBEsol	PBE−D2	PBE−D3	revM06−L	revTPSS	SCAN	SOGGA	vdW−DF2
$Co_2C_8N_{12}$	N-Co-N	88.95	88.71	89.28	88.99	89.02	89.03	88.96	88.99	88.99	89.47	89.12
		85.14	86.29	87.26	85.48	85.68	86.02	84.95	91.00	85.10	85.53	86.64
		91.05	91.29	90.71	91.00	90.97	90.97	91.04	91.09	91.00	90.53	90.87
		94.86	93.58	93.75	94.51	93.99	94.17	94.55	93.66	94.11	94.58	93.35
$Cu_3H_4C_{10}O_{10}$	O-Cu-O	94.86	93.58	93.75	94.51	93.99	94.17	94.55	93.66	94.11	94.58	93.35
		95.57	97.28	95.05	96.12	95.50	95.48	95.91	96.55	96.26	94.76	96.9
		95.48	95.27	98.10	96.56	96.38	96.95	95.70	96.48	96.35	96.46	98.97
		82.83	81.81	79.95	81.33	82.02	82.29	82.71	81.18	81.45	83.04	80.04
		89.53	89.21	90.56	89.21	89.78	89.20	89.20	89.44	90.19	89.58	89.31
$Cu_8H_8C_8N_{12}Cl_8$	N-Cu-Cl	89.32	88.29	90.38	89.84	88.52	89.52	89.50	89.72	89.57	91.46	89.4
		90.68	91.70	89.61	90.15	91.47	90.47	90.49	90.27	90.42	88.53	90.59
$Dy_2H_{12}C_{12}N_2O_{16}$	O-Dy-O	75.84	80.49	78.84	79.90	82.84	79.84	78.03	78.12	79.06	80.17	79.87
		75.51	75.05	77.85	78.05	75.90	76.75	76.19	77.21	76.69	78.13	76.29
		73.54	68.04	76.14	75.20	69.36	72.34	73.00	74.74	73.22	75.01	71.69
		74.21	77.77	71.81	71.08	71.76	72.44	73.78	71.96	72.49	70.64	73.4
		80.01	86.18	75.70	76.55	82.74	78.72	79.45	76.65	79.23	76.68	80.64
		85.78	82.72	84.41	85.04	87.51	84.91	84.89	84.33	85.70	84.91	84.42
		83.15	77.30	87.43	86.96	82.89	84.78	82.22	85.47	83.69	86.74	83.42
		76.09	75.61	76.79	76.30	76.93	76.71	75.60	77.44	76.33	76.04	74.98
$Fe_4H_4C_4O_{12}$	O-Fe-O	88.31	93.68	85.09	84.70	83.16	85.52	88.11	86.45	91.95	84.006	84.79
		73.86	79.31	71.75	73.86	71.51	74.61	72.91	77.18	72.98	82.002	81.89
		85.59	84.94	83.73	83.14	82.64	83.60	84.69	84.79	82.21	73.28	79.51
		104.87	98.64	98.73	100.22	98.16	107.91	106.67	106.62	103.09	106.96	102.13
		87.34	89.35	90.41	89.32	88.82	88.94	86.20	89.18	85.264	82.25	84.76
		93.86	90.08	92.34	92.33	92.03	92.58	89.31	91.91	84.15	91.73	91.59
$Fe_4P_4H_{16}C_8O_{24}$	O-Fe-O	94.16	92.87	94.21	94.61	94.48	94.72	93.24	93.87	94.23	94.06	94.43
		81.65	81.32	81.07	82.41	82.59	81.50	80.78	81.28	81.54	81.97	81.19
		84.39	86.46	83.12	87.93	87.34	83.97	84.22	83.32	84.65	83.99	82.98
		90.43	92.72	89.23	90.89	91.01	89.96	89.62	89.71	90.54	89.28	93.18
		93.43	91.09	94.70	92.50	91.77	93.38	94.53	94.19	93.40	94.29	91.85
		90.84	85.37	92.39	90.33	89.99	90.53	90.66	91.82	90.08	90.89	89.5
		78.47	81.75	76.3	73.29	74.87	74.84	78.54	73.88	79.88	72.95	83.68
		152.01	154.95	151.92	151.05	154.89	148.84	151.37	151.03	151.07	149.11	157.07
		161.34	164.49	164.71	162.51	165.83	158.57	161.26	158.07	164.96	163.21	165.53
		174.05	175.6	174.99	171.36	178.03	168.62	172.36	171.73	172.03	174.46	168.95
		87.09	87.33	87.52	82.09	82.05	84.6	85.72	88.40	85.61	83.09	82.99
		88.92	92.21	87.9	89.92	86.58	91.21	90.35	92.88	90.32	89.88	96.39
		120.59	119.68	123.46	123.57	123.79	122.9	121.29	119.19	124.08	123.17	125.68
$Sm_2H_{12}C_{10}O_{14}$	O-Sm-O	51.02	51.96	51.32	51.88	51.34	51.49	51.00	51.79	51.68	52.03	51.34
		75.42	76.97	74.56	73.86	74.16	74.19	76.63	73.90	74.94	73.82	74.24
		77.21	69.06	74.54	75.28	77.18	75.80	70.28	74.42	77.40	75.35	78.25
		75.97	65.62	74.06	75.56	77.42	75.33	69.86	75.10	76.87	75.50	76.93
		74.86	79.17	77.73	75.75	73.69	77.23	78.50	76.19	73.61	75.61	76.93
		67.35	71.30	65.91	66.30	69.55	66.70	68.71	66.08	66.83	66.10	68.83
UiO-66	Zr-O-Zr	112.76	112.76	110.40	110.21	110.08	112.76	112.8	112.76	116.50	110.04	110.69
	O-Zr-O	77.30	77.30	76.09	76.02	75.92	71.03	81.38	77.30	81.69	75.91	76.41
MOF-5	Zn-O-Zn	109.47	109.47	109.47	109.47	109.47	109.47	109.55	109.47	109.47	109.47	109.47
	O-Zn-O	106.36	106.36	107.34	107	107.35	107.40	108.47	107.09	106.87	106.93	107.59
MSE (°)			**0.10**	**0.06**	**-0.34**	**-0.11**	**-0.05**	**-0.02**	**-0.43**	**0.01**	**-0.42**	0.26
MUE (°)			**2.46**	**2.00**	**1.71**	**1.75**	**1.15**	**1.20**	**1.94**	**1.19**	**1.95**	1.77
MUPE (%)			**2.74**	**2.18**	**1.81**	**1.84**	**1.33**	**1.31**	**1.93**	**1.26**	**2.13**	**1.87**

[a] The references for the experimental bond angles are given in Table S1.

Table S7: Torsional angles (deg) of the metal–organic frameworks (MOFs) calculated using various local and meta functionals.

MOF	Torsional angle type	Exp.[a]	MN15-L	PBE	PBEsol	PBE–D2	PBE–D3	revM06-L	revTPSS	SCAN	SOGGA	vdW-DF2
$Ag_4C_{12}Cl_4O_8$	Ag-O-Ag-Cl	142.58	134.67	132.45	125.89	158.72	135.42	135.01	122.88	137.23	125.78	139.92
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	N-Cd-N-C	140.60	141.83	145.95	142.96	142.99	142.99	141.05	143.43	143.47	143.06	143.55
$Cd_2H_{10}C_{16}N_4O_{10}$	O-Cd-N-C	123.80	123.43	127.59	124.03	124.03	124.37	123.73	124.06	124.09	123.92	126.52
$Zn_1H_4C_4O_4$	O-Zn-O-C	151.50	169.98	144.71	144.12	145.99	150.26	146.89	143.42	150.02	144.12	157.51
$Li_8Zn_8H_{24}C_{72}O_{48}$	Li-O-Zn-O	128.40	127.80	130.29	127.96	131.39	130.04	128.33	125.71	127.73	127.96	133.44
$Co_2C_8N_{12}$	N-Co-N-C	150.30	166.86	164.66	148.88	154.73	154.11	150.42	150.76	149.66	171.06	161.48
$Cu_3H_4C_{10}O_{10}$	Cu-O-Cu-O	117.64	116.81	129.2	119.02	118.91	123.86	117.28	119.54	122.23	118.90	121.03
$Cu_8H_8C_8N_{12}Cl_8$	Cu-Cl-Cu-Cl	153.40	149.82	157.94	152.41	153.85	152.65	151.65	152.69	153.17	148.36	141.86
$Dy_2H_{12}C_{12}N_2O_{16}$	O-Dy-O-C	165.23	173.83	174.61	167.66	173.46	169.97	168.08	168.05	169.91	167.79	171.28
$Fe_4H_4C_4O_{12}$	O-Fe-O-C	164.70	168.11	162.02	170.05	163.33	169.84	159.21	164.91	165.53	158.15	171.83
$Fe_4P_4H_{16}C_8O_{24}$	Fe-O-P-O	93.40	93.48	101.52	102.58	120.05	105.31	89.73	94.37	94.19	95.03	102.22
$Sm_2H_{12}C_{10}O_{14}$	O-Sm-O-C	131.55	126.77	141.87	136.30	134.43	134.57	127.74	136.71	132.35	136.34	136.67
UiO-66	Zr-O-Zr-O	154.96	154.96	157.87	158.09	158.21	154.96	156.96	154.96	150.11	158.26	157.66
MOF-5	Zn-O-Zn-O	120	120	120	120	120	120	120	120	120	120	120
MSE (°)			**2.16**	**3.75**	**0.13**	**4.43**	**2.16**	**-1.57**	**-0.96**	**0.11**	**-0.05**	**3.35**
MUE (°)			**4.74**	**6.55**	**3.98**	**5.41**	**3.47**	**2.34**	**3.48**	**2.00**	**5.22**	**5.37**
MUPE (%)			**3.17**	**4.85**	**2.98**	**4.43**	**2.76**	**1.67**	**2.47**	**1.42**	**3.57**	**3.92**

[a] The references for the experimental bond lengths are given in Table S1.

Table S8: Lattice angles (deg) of the metal–organic frameworks (MOFs) calculated using various local and meta functionals.

MOF	Exp.[a]	MN15−L	PBE	PBEsol	PBE−D2	PBE−D3	revM06−L	revTPSS	SCAN	SOGGA	vdW−DF2
$Ag_4C_{12}Cl_4O_8$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=86.73	β=97.92	β=94.99	β=89.59	β=91.30	β=90.97	β=96.02	β=91.33	β=95.19	β=91.53
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Cd_{12}H_{48}C_{72}N_{72}O_{48}$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Cd_2H_{10}C_{16}N_4O_{10}$	α=71.4	α=72.6	α=70.18	α=70.40	α=69.73	α=70.06	α=71.98	α=71.00	α=70.94	α=70.39	α=70.53
	β=73	β=76	β=71.85	β=71.97	β=72.57	β=72.37	β=74.20	β=72.26	β=72.75	β=71.96	β=73.15
	γ=74.9	γ=77.14	γ=74.36	γ=73.73	γ=73.81	γ=73.77	γ=75.19	γ=74.49	γ=74.24	γ=73.74	γ=74.27
$Zn_1H_4C_4O_4$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=108.5	β=110.65	β=*11*4.42	β=*10*4.64	β=*105*.35	β=*105*.83	β=*10*4.28	β=*11*0.92	β=*105*.23	β=*10*4.62	β=*10*4.52
	γ=90	γ=90	γ=*90*	γ=*90*	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Li_8Zn_8H_{24}C_{72}O_{48}$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
UiO-66	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
MOF-5	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Co_2C_8N_{12}$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Cu_3H_4C_{10}O_{10}$	α=98.6	α=100.43	α=96.91	α=98.99	α=99.17	α=98.17	α=99.44	α=98.48	α=99.00	α=*108.78*	α=98.91
	β=92	β=91.99	β=91.40	β=92.02	β=92.04	β=91.74	β=92.32	β=91.85	β=92.02	β=97.90	β=91.86
	γ=94.3	γ=93.61	γ=96.98	γ=94.95	γ=95.39	γ=95.47	γ=94.39	γ=95.00	γ=95.62	γ=90.93	γ=94.87
$Cu_8H_8C_8N_{12}Cl_8$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Dy_2H_{12}C_{12}N_2O_{16}$	α=95.6	α=96.49	α=90	α=96.12	α=95.13	α=95.89	α=*95.60*	α=96.07	α=95.67	α=96.19	α=95.49
	β=110.4	β=108.38	β=90	β=109.51	β=113.12	β=111.50	β=111.62	β=*109.38*	β=111.24	β=109.36	β=111.77
	γ=94.5	γ=93.65	γ=90	γ=93.69	γ=93.73	γ=94.28	γ=94.43	γ=*94.03*	γ=94.05	γ=93.78	γ=94.43
$Fe_4H_4C_4O_{12}$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90.6	β=71.88	β=90	β=92.53	β=90	β=90.59	β=90.59	β=90	β=88.68	β=72.30	β=89.75
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Fe_4P_4H_{16}C_8O_{24}$	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90	α=90
	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90	β=90
	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90	γ=90
$Sm_2H_{12}C_{10}O_{14}$	α=101.9	α=103.32	α=101.47	α=101.32	α=99.95	α=100.61	α=102.17	α=101.89	α=101.41	α=103.13	α=101.22
	β=103.1	β=102.78	β=101.62	β=101.89	β=102.29	β=102.21	β=104.11	β=102.32	β=103.13	β=99.57	β=103.25
	γ=101.4	γ=98.21	γ=103.20	γ=103.44	γ=101.87	γ=102.45	γ=99.15	γ=*10*2.87	γ=101.81	γ=97.12	γ=100.86
MSE		**-0.38**	**-0.48**	**-0.0005**	**-0.13**	**-0.09**	**0.008**	**0.15**	**-0.07**	**-0.20**	**-0.08**
MUE		**0.99**	**1.34**	**0.49**	**0.37**	**0.32**	**0.31**	**0.37**	**0.28**	**1.26**	**0.28**
MUPA (%)		**2.38**	**1.35**	**2.25**	**1.52**	**3.52**	**0.32**	**0.40**	**0.29**	**1.36**	**0.29**

Table S9: Lattice constants and band gaps of ten semiconductors calculated with the revM06-L and SCAN functionals

Systems	Experimental[a]		revM06-L		SCAN	
	Lattice Constants (Å)	**Band Gaps (eV)**	**Lattice Constants (Å)**	**Band Gaps (eV)**	**Lattice Constants (Å)**	**Band Gaps (eV)**
Si	*a*=*b*=*c*= 5.430	1.17	5.430	1.10	5.423	0.95
Ge	*a*=*b*=*c*= 5.657	0.74	5.707	1.13	5.687	1.13
SiC	*a*=*b*=*c*= 4.348	2.42	4.319	2.35	4.348	1.87
β-GaN	*a*=*b*=*c*= 4.545	3.30	4.514	2.61	4.523	2.27
CdS	*a*=*b*=*c*= 5.818	2.55	5.909	2.34	5.879	1.68
CdSe	*a*=*b*=*c*= 6.213	1.90	6.172	1.67	6.134	1.12
ZnS	*a*=*b*=*c*= 5.409	3.66	5.387	3.45	5.375	2.74
ZnO	*a*=*b*=3.249 *c*=5.207	3.40	*a*=*b*=3.189 *c*=5.162	1.87	*a*=*b*=3.234 *c*=5.224	1.73
TiO_2 (anatase)[b]	*a*=*b*=3.803 *c*=9.748 (18)	3.20 (19)	*a*=*b*=3.802 *c*=9.590	2.56	*a*=*b*=3.797 *c*=9.547	2.27
TiO_2 (rutile)[b]	*a*=*b*=4.653 *c*=2.969 (18)	3.00 (20)	*a*=*b*=4.621 *c*=2.961	2.19	*a*=*b*=4.622 *c*=2.951	1.90
MSE			–0.01	–0.40	–0.05	–0.77
MUE			0.05	0.48	0.04	0.85
MUPE			**0.68**	**19.54**	**0.57**	**48.96**

[a] The experimental lattice constants are taken from the LC17 database[21] and the band gaps are taken from the SBG31 database[21] except for the anatase and rutile phases of TiO_2.

[b] The references for the experimental lattice constants and band gaps of TiO_2 (anatase and rutile) are given in the parentheses after the experimental values.

[c] MSE: mean signed error; MUE: mean unsigned error; MUPE: mean unsigned percentage error.

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