Supplementary Information for

Benchmarking Quantum Chemistry Predictions of Framework Structures and Properties in a Chemically Diverse Test Set of Metal Organic Frameworks

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Table S 1: MOF primitive unit cell size and computational parameter setup. An energy cut off of 520 eV was used for all calculations.

REFCODE	Chemical Formula	Experimental Lattice Parameters (Å)			kpoints	Comments
		a	b	c		
QEJZUB01[1]	$Cu_3H_4C_{10}O_{10}$	6.77	6.89	12.36	4 x 4 x 2	
HOGWAB[2]	$Fe_4H_4C_4O_{12}$	5.54	5.93	7.27	4 x 4 x 4	
HAWVOQ01[3]	$Co_2C_8N_{12}$	5.97	7.06	7.41	4 x 4 x 4	
RORQOE[4]	$Ag_4C_{12}C_{l4}O_8$	5.29	6.34	11.40	6 x 4 x 2	
OFUWIV01[5]	$Zn_1H_4C_4O_4$	4.83	4.83	6.25	6 x 6 x 4	
MURCEH[6]	$Cu_8H_8C_8N_{12}Cl_8$	5.02	5.81	19.25	4 x 4 x 2	Antiferromagnetic: see below for spin states for each metal
WAJJAU[7]	$Li_{32}Zn_{32}H_{24}C_{72}O_{96}$	11.28	16.34	16.34	2 x 2 x 2	For PBE-D2 (Li: C6 = 31.47 $\frac{Jnm^6}{mol}$ R0 = 2.077 Å)
PIJGEV[8]	$Cd_2H_{10}C_{16}N_4O_{10}$	7.55	7.64	8.47	4 x 4 x 4	
KOMJEC[9]	$Sm_2H_{12}C_{10}O_{14}$	6.76	7.67	8.05	4 x 4 x 4	For PBE-D2 (Sm: C6 =33.98 $\frac{Jnm^6}{mol}$ R0 = 2.226 Å)
YORSII[10]	$Dy_2H_{12}C_{12}N_2O_{16}$	6.74	7.81	9.17	4 x 4 x 2	
DEMLIR[11]	$Fe_4P_4H_{16}C_8O_{24}$	6.61	8.36	9.62	4 x 4 x 2	Antiferromagnetic: see below for spin states for each metal

Fractional coordinates of Cu atoms and corresponding initial spin state in MURCEH

0.000000000	0.500000000	0.500000000	-2
0.000000000	0.500000000	0.000000000	-2
0.812179983	0.957530022	0.437770009	2
0.812179983	0.957530022	0.937770009	2
0.187820002	0.042470001	0.062229998	-2
0.187820002	0.042470001	0.562229991	2

Fractional coordinates of Fe atoms and corresponding initial spin state in DEMLIR

0.023400	0.511260	0.402520	2
0.476600	0.488740	0.902520	-2
0.976600	0.011260	0.097480	-2
0.523400	0.988740	0.597480	2

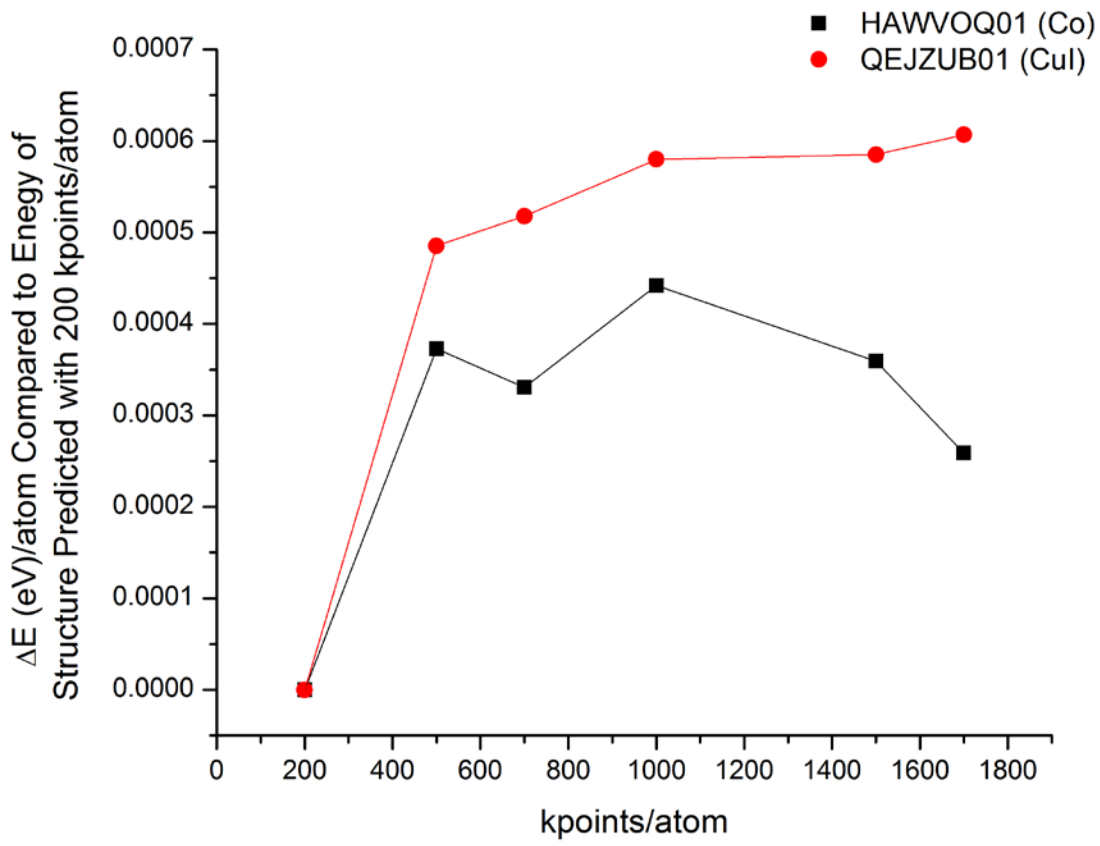

Figure S 2: HAWVOQ01 and QEJZUB01, with metal centers of Co and CuI, respectively were analyzed for change in predicted energy per atom with increase in kpoint density. The PBE-D2 functional was used. We find that after 1000 kpoints/atom, the predicted energies are within the convergence criteria of 0.0001 eV.

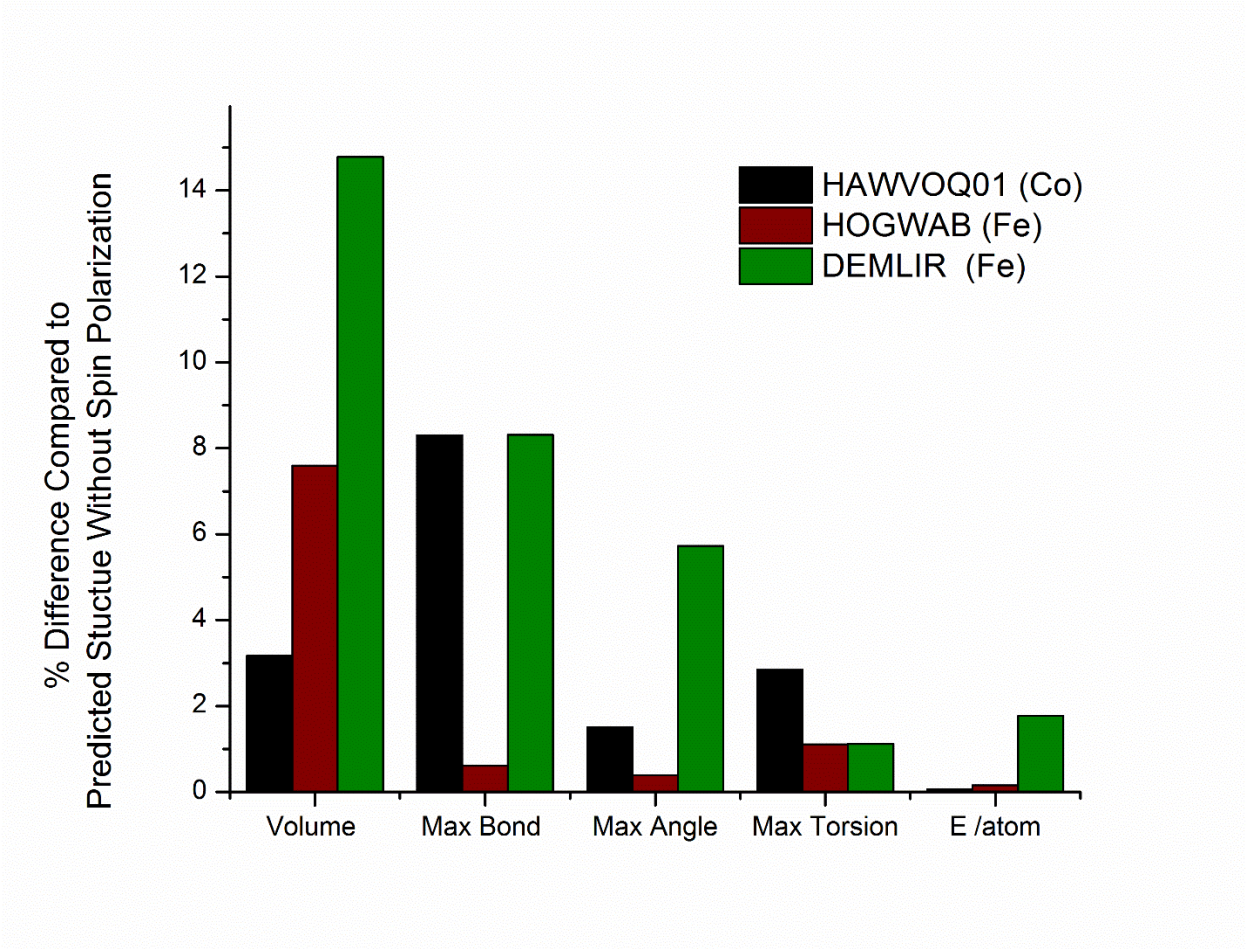

Figure S 3: HAWVOQ01, HOGWAB, and anti-ferromagnetic DEMLIR with magnetic centers, Co, Fe, and Fe, respectively, were analyzed for change in volume, the geometry of the local metal center environment (bond length, bond angle, and torsion angle) and ground state energy. The results are shown as magnitude of percent change compared to structures predicted without spin polarization. The PBE functional was used.

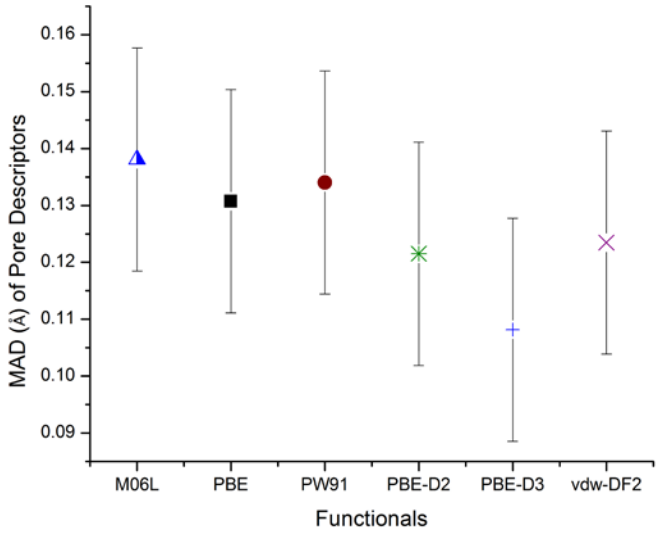

Figure S 4: MAD of PLDs and LCDs for all MOFs in test set

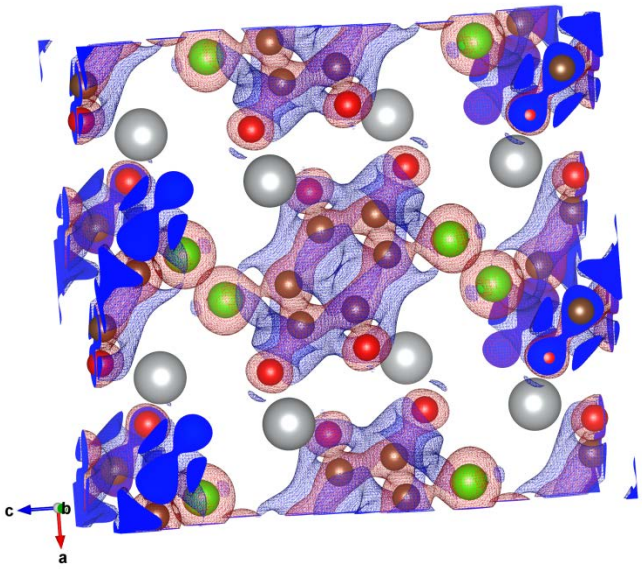

Figure S 5: Charge density difference isosurfaces between vdw-DF2 and PBE for the experimental structure of RORQOE MOF. (Ag: silver, C: brown, O: red, Cl: green). Isosurfaces plotted at 0.002 electrons/ bohr^3 with red indicating a positive and blue a negative difference. Slightly higher oxygen and chlorine density is predicted for oxygen with vdw-DF2 than PBE. When the structure of RORQOE energy is minimized, vdw-DF2 predicts a more accurate, 10° smaller, Cl-Ag-O bond angle then PBE.

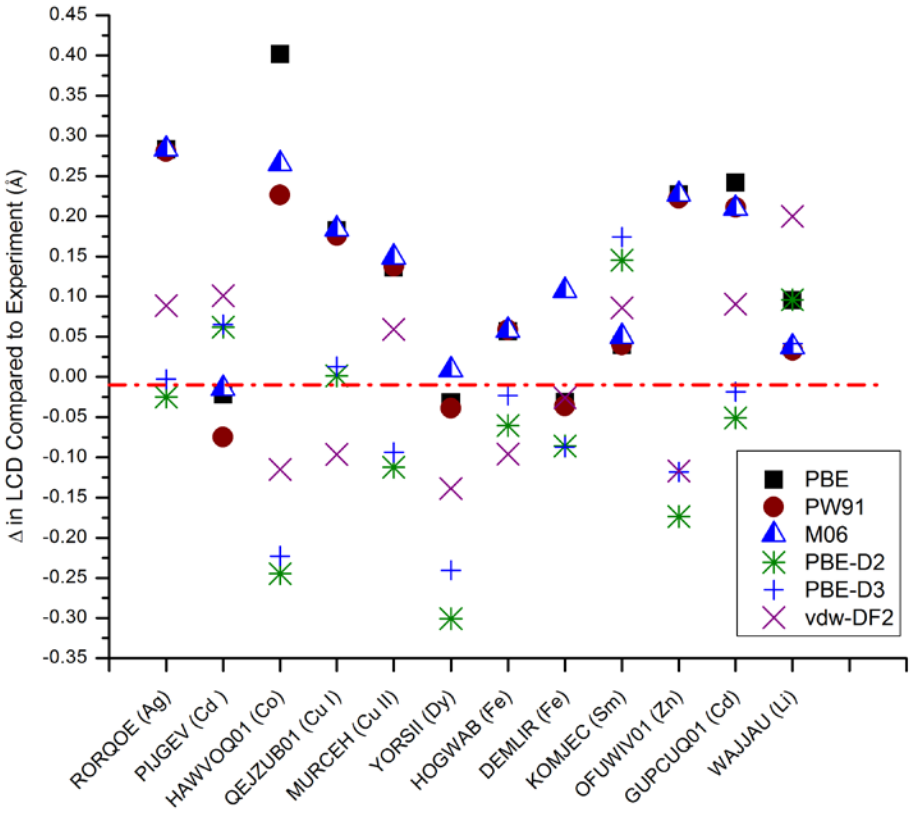

Figure S 6: Deviation of LCD from experimental structure.

Table S 2: MAD of Δ in lattice parameters (Å) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**0.59**	**0.58**	**0.57**	**0.27**	**0.02**	**0.20**
PIJGEV (Cd)	**0.25**	**0.25**	**0.20**	**0.03**	**0.07**	**0.16**
HAWVOQ01 (Co)	**0.37**	**0.41**	**0.42**	**0.21**	**0.18**	**0.09**
QEJZUB01 (Cu I)	**0.24**	**0.24**	**0.24**	**0.11**	**0.16**	**0.16**
MURCEH (Cu II)	**0.16**	**0.17**	**0.16**	**0.05**	**0.07**	**0.21**
YORSII (Dy)	**0.12**	**0.15**	**0.11**	**0.04**	**0.05**	**0.11**
HOGWAB (Fe)	**0.17**	**0.17**	**0.18**	**0.08**	**0.06**	**0.23**
DEMLIR (Fe)	**0.15**	**0.12**	**0.13**	**0.21**	**0.21**	**0.06**
KOMJEC (Sm)	**0.18**	**0.18**	**0.18**	**0.09**	**0.06**	**0.12**
OFUWIV01 (Zn)	**0.16**	**0.16**	**0.16**	**0.03**	**0.09**	**0.10**
GUPCUQ01 (Cd)	**0.30**	**0.30**	**0.28**	**0.10**	**0.14**	**0.32**
WAJJAU (Li Zn)	**0.14**	**0.16**	**0.16**	**0.07**	**0.06**	**0.40**

Table S 3: MAD of Δ in bond length (Å) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**0.076**	**0.074**	**0.064**	**0.028**	**0.015**	**0.078**
PIJGEV (Cd)	**0.062**	**0.062**	**0.055**	**0.022**	**0.033**	**0.077**
HAWVOQ01 (Co)	**0.213**	**0.208**	**0.203**	**0.186**	**0.198**	**0.182**
QEJZUB01 (Cu I)	**0.112**	**0.112**	**0.109**	**0.051**	**0.050**	**0.064**
MURCEH (Cu II)	**0.032**	**0.028**	**0.035**	**0.009**	**0.014**	**0.064**
YORSII (Dy)	**0.024**	**0.035**	**0.023**	**0.022**	**0.025**	**0.045**
HOGWAB (Fe)	**0.085**	**0.085**	**0.083**	**0.052**	**0.051**	**0.030**
DEMLIR (Fe)	**0.033**	**0.065**	**0.068**	**0.075**	**0.076**	**0.036**
KOMJEC (Sm)	**0.026**	**0.027**	**0.026**	**0.011**	**0.015**	**0.056**
OFUWIV01 (Zn)	**0.038**	**0.038**	**0.034**	**0.023**	**0.041**	**0.054**
GUPCUQ01 (Cd)	**0.051**	**0.053**	**0.047**	**0.023**	**0.032**	**0.080**
WAJJAU (Li Zn)	**0.029**	**0.024**	**0.028**	**0.023**	**0.021**	**0.073**

Table S 4: MAD of Δ in bond angle (°) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**4.76**	**4.72**	**4.78**	**3.67**	**0.55**	**1.48**
PIJGEV (Cd)	**2.14**	**2.08**	**1.80**	**1.17**	**1.17**	**0.65**
HAWVOQ01 (Co)	**0.93**	**0.95**	**0.98**	**0.36**	**0.44**	**0.64**
QEJZUB01 (Cu I)	**2.95**	**2.96**	**2.88**	**0.77**	**0.53**	**2.60**
MURCEH (Cu II)	**1.82**	**1.85**	**2.39**	**1.06**	**0.91**	**1.37**
YORSII (Dy)	**1.95**	**2.07**	**2.01**	**2.15**	**1.37**	**1.20**
HOGWAB (Fe)	**1.88**	**1.88**	**2.14**	**3.43**	**3.13**	**5.17**
DEMLIR (Fe)	**1.09**	**1.62**	**1.73**	**1.97**	**1.94**	**1.74**
KOMJEC (Sm)	**2.40**	**2.34**	**2.40**	**1.32**	**1.17**	**1.50**
OFUWIV01 (Zn)	**2.24**	**2.24**	**2.35**	**0.86**	**1.01**	**0.97**
GUPCUQ01 (Cd)	**0.52**	**0.74**	**0.47**	**1.35**	**1.40**	**2.39**
WAJJAU (Li Zn)	**0.83**	**0.69**	**0.56**	**0.99**	**1.02**	**1.39**

Table S 5: MAD of Δ in torsion angle (°) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**9.37**	**9.27**	**9.39**	**7.28**	**1.06**	**2.21**
PIJGEV (Cd)	**5.78**	**5.67**	**4.86**	**3.91**	**2.84**	**2.42**
HAWVOQ01 (Co)	**11.21**	**14.73**	**13.24**	**8.13**	**7.72**	**6.79**
QEJZUB01 (Cu I)	**6.18**	**3.95**	**5.83**	**7.87**	**7.55**	**5.94**
MURCEH (Cu II)	**12.90**	**11.38**	**6.73**	**12.93**	**8.11**	**11.63**
YORSII (Dy)	**8.54**	**8.58**	**8.85**	**6.57**	**7.14**	**5.09**
HOGWAB (Fe)	**2.15**	**2.15**	**2.80**	**4.78**	**4.30**	**7.92**
DEMLIR (Fe)	**3.43**	**8.78**	**8.79**	**11.48**	**10.74**	**8.98**
KOMJEC (Sm)	**10.87**	**10.83**	**10.87**	**4.17**	**3.95**	**5.62**
OFUWIV01 (Zn)	**5.05**	**5.05**	**4.92**	**2.78**	**2.83**	**4.20**
GUPCUQ01 (Cd)	**1.14**	**1.27**	**1.08**	**1.63**	**1.75**	**2.16**
WAJJAU (Li Zn)	**1.52**	**1.83**	**1.70**	**1.44**	**1.27**	**4.04**

Table S 6: Δ in PLD (Å) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**0.20**	**0.20**	**0.20**	**-0.20**	**-0.01**	**0.13**
PIJGEV (Cd)	**0.13**	**0.13**	**0.06**	**0.01**	**-0.03**	**-0.01**
HAWVOQ01 (Co)	**0.33**	**0.20**	**0.36**	**-0.30**	**-0.28**	**-0.22**
QEJZUB01 (Cu I)	**0.11**	**0.11**	**0.10**	**-0.11**	**-0.10**	**-0.25**
MURCEH (Cu II)	**0.15**	**0.16**	**0.16**	**-0.03**	**0.02**	**0.08**
YORSII (Dy)	**0.14**	**0.15**	**0.15**	**-0.03**	**0.02**	**0.07**
HOGWAB (Fe)	**-0.17**	**-0.18**	**-0.17**	**-0.32**	**-0.32**	**-0.41**
DEMLIR (Fe)	**0.06**	**-0.10**	**-0.11**	**-0.23**	**-0.20**	**-0.13**
KOMJEC (Sm)	**0.09**	**0.09**	**0.09**	**-0.15**	**-0.13**	**-0.09**
OFUWIV01 (Zn)	**0.18**	**0.18**	**0.18**	**-0.11**	**-0.05**	**-0.05**
GUPCUQ01 (Cd)	**0.07**	**0.08**	**0.08**	**-0.02**	**-0.01**	**-0.01**
WAJJAU (Li Zn)	**0.04**	**0.01**	**0.03**	**-0.04**	**-0.08**	**0.22**

Table S 7: Δ in LCD (Å) by MOF

	M06L	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**0.28**	**0.28**	**0.28**	**-0.03**	**0.00**	**0.09**
PIJGEV (Cd)	**-0.01**	**-0.02**	**-0.07**	**0.06**	**0.07**	**0.10**
HAWVOQ01 (Co)	**0.27**	**0.40**	**0.23**	**-0.24**	**-0.22**	**-0.11**
QEJZUB01 (Cu I)	**0.18**	**0.18**	**0.18**	**0.00**	**0.01**	**-0.10**
MURCEH (Cu II)	**0.15**	**0.14**	**0.14**	**-0.11**	**-0.09**	**0.06**
YORSII (Dy)	**0.01**	**-0.03**	**-0.04**	**-0.30**	**-0.24**	**-0.14**
HOGWAB (Fe)	**0.06**	**0.06**	**0.06**	**-0.06**	**-0.02**	**-0.10**
DEMLIR (Fe)	**0.11**	**-0.03**	**-0.04**	**-0.09**	**-0.09**	**-0.03**
KOMJEC (Sm)	**0.05**	**0.04**	**0.04**	**0.15**	**0.17**	**0.09**
OFUWIV01 (Zn)	**0.23**	**0.23**	**0.22**	**-0.17**	**-0.12**	**-0.12**
GUPCUQ01 (Cd)	**0.21**	**0.24**	**0.21**	**-0.05**	**-0.02**	**0.09**
WAJJAU (Li Zn)	**0.04**	**0.10**	**0.03**	**0.10**	**0.04**	**0.20**

Table S 8: Angles of the experimental crystal structures considered for three example MOFs in the test set.

HOGWAB				**RORQOE**				**HAWVOQ01**			
O	Fe	O	78.47	Cl	Ag	O	68.37	N	Co	N	94.86
O	Fe	O	73.86	Cl	Ag	O	74.94	N	Co	N	85.14
O	Fe	O	88.31	Cl	Ag	O	135.63	N	Co	N	91.05
O	Fe	O	161.34	Cl	Ag	O	137.90	N	Co	N	88.95
O	Fe	O	87.09	O	Ag	O	110.23				
O	Fe	O	152.01	O	Ag	O	108.82				
O	Fe	O	93.86	O	Ag	O	139.57				
O	Fe	O	87.34	O	Ag	O	137.82				
O	Fe	O	88.92	O	Ag	O	65.96				
O	Fe	O	89.51	O	Ag	O	74.16				
O	Fe	O	120.59								
O	Fe	O	85.59								
O	Fe	O	80.54								
O	Fe	O	174.05								
O	Fe	O	104.87								

Our studies show that results for the mechanical properties for DEMLIR are sensitive to the number of processors used for the calculations. Each calculation for DEMLIR has been tested along four differently compiled versions of VASP, using version 5.2.12 and 5.3.5 and two different computing environments. We've found that result are reproducible as long as the same number of processors are used. Energy and geometry optimization calculations are not effected by parallelization. For our study, DEMLIR mechanical properties were calculated using 32 processors.

Table S 9: Minimum Young's modulus for MOFs in the test set (GPa)

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**22.7**	**19.6**	**20.7**	**16.5**	**17.1**	**17.9**
PIJGEV (Cd)	**102.1**	**98.1**	**99.4**	**96.6**	**100.3**	**103.7**
HAWVOQ01 (Co)	**23.2**	**19.0**	**21.8**	**21.4**	**20.7**	**17.2**
QEJZUB01 (Cu I)	**46.1**	**36.3**	**36.5**	**35.0**	**33.9**	**40.8**
MURCEH (Cu II)	**48.1**	**48.2**	**48.6**	**48.3**	**48.2**	**47.1**
YORSII (Dy)	**143.9**	**141.4**	**141.5**	**140.5**	**140.8**	**150.2**
HOGWAB (Fe)	**67.0**	**67.7**	**67.9**	**64.8**	**66.4**	**81.2**
DEMLIR (Fe)	**184.9**	**185.1**	**168.3**	**184.2**	**184.2**	**179.6**
KOMJEC (Sm)	**146.0**	**145.0**	**145.0**	**141.1**	**144.4**	**156.4**
OFUWIV01 (Zn)	**111.4**	**110.2**	**110.7**	**110.4**	**111.4**	**110.4**

Table S 10: Maximum Young's modulus for MOFs in the test set (GPa)

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**284.9**	**281.4**	**284.5**	**282.5**	**283.4**	**285.3**
PIJGEV (Cd)	**406.7**	**403.5**	**403.2**	**401.7**	**404.7**	**405.4**
HAWVOQ01 (Co)	**482.1**	**461.2**	**466.8**	**464.9**	**468.6**	**461.4**
QEJZUB01 (Cu I)	**361.3**	**359.5**	**353.7**	**361.8**	**354.9**	**362.8**
MURCEH (Cu II)	**430.7**	**425.4**	**428.3**	**425.1**	**434.2**	**437.9**
YORSII (Dy)	**340.7**	**340.2**	**339.9**	**337.3**	**337.9**	**343.1**
HOGWAB (Fe)	**461.4**	**460.1**	**460.8**	**461.9**	**453.3**	**468.5**
DEMLIR (Fe)	**351.1**	**352.8**	**339.5**	**354.2**	**354.2**	**342.8**
KOMJEC (Sm)	**432.0**	**431.4**	**431.4**	**427.8**	**431.3**	**430.6**
OFUWIV01 (Zn)	**379.3**	**380.4**	**379.8**	**380.6**	**380.2**	**376.6**

Table S 11: Minimum linear compressibility for MOFs in the test set (TPa^{-1})

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**-20.6**	**-25.3**	**-23.4**	**-31.1**	**-29.9**	**-28.5**
PIJGEV (Cd)	**0.7**	**0.7**	**0.7**	**0.7**	**0.7**	**0.8**
HAWVOQ01 (Co)	**-3**	**-3.6**	**-3.4**	**-3.5**	**-3.5**	**-3.2**
QEJZUB01 (Cu I)	**1.1**	**1.2**	**1.3**	**1.2**	**1.4**	**1.1**
MURCEH (Cu II)	**0.9**	**1.1**	**0.9**	**1.1**	**0.9**	**0.9**
YORSII (Dy)	**1.1**	**1.1**	**1.1**	**1.1**	**1.1**	**1.1**
HOGWAB (Fe)	**1.0**	**1.0**	**1.0**	**0.9**	**1.0**	**1.1**
DEMLIR (Fe)	**0.9**	**0.8**	**1.027**	**0.8**	**0.8**	**0.9**
KOMJEC (Sm)	**0.8**	**0.7**	**0.7**	**0.7**	**0.8**	**0.8**
OFUWIV01 (Zn)	**1.0**	**1.0**	**1.0**	**1.0**	**1.0**	**1.0**

Table S 12: Maximum linear compressibility for MOFs in the test set (TPa^{-1})

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**31.7**	**38**	**36.1**	**46**	**44.4**	**40.3**
PIJGEV (Cd)	**5.6**	**5.9**	**5.8**	**6**	**5.7**	**5.4**
HAWVOQ01 (Co)	**21.2**	**26.2**	**22.9**	**24.5**	**25**	**25**
QEJZUB01 (Cu I)	**11.1**	**14**	**13.2**	**15.1**	**15**	**10.8**
MURCEH (Cu II)	**3.6**	**3.5**	**3.6**	**3.6**	**3.7**	**3.4**
YORSII (Dy)	**4.3**	**4.4**	**4.4**	**4.4**	**4.4**	**4**
HOGWAB (Fe)	**10.8**	**10.4**	**10.4**	**11**	**10.8**	**8.6**
DEMLIR (Fe)	**2.6**	**2.5**	**3.1**	**2.6**	**2.6**	**2.8**
KOMJEC (Sm)	**3.6**	**3.6**	**3.6**	**3.7**	**3.6**	**3.3**
OFUWIV01 (Zn)	**4.4**	**4.5**	**4.5**	**4.4**	**4.4**	**4.4**

Table S 13: Minimum shear modulus for MOFs in the test set (GPa)

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**7.5**	**6.4**	**6.9**	**5.4**	**5.6**	**5.7**
PIJGEV (Cd)	**43.4**	**42.3**	**42.7**	**41.7**	**43.0**	**44.6**
HAWVOQ01 (Co)	**8.6**	**7.3**	**8.2**	**8.3**	**8.0**	**6.1**
QEJZUB01 (Cu I)	**14.0**	**10.9**	**10.9**	**10.6**	**10.2**	**12.0**
MURCEH (Cu II)	**15.1**	**15.3**	**15.3**	**15.2**	**15.2**	**14.9**
YORSII (Dy)	**60.2**	**59.5**	**59.5**	**59.2**	**59.6**	**62.2**
HOGWAB (Fe)	**35.3**	**35.0**	**35.2**	**34.1**	**34.8**	**40.1**
DEMLIR (Fe)	**79.2**	**79.1**	**72.2**	**79.4**	**79.4**	**76.1**
KOMJEC (Sm)	**56.2**	**55.8**	**55.8**	**54.3**	**55.6**	**59.1**
OFUWIV01 (Zn)	**44.5**	**44.4**	**44.5**	**44.1**	**44.5**	**43.4**

Table S 14: Maximum shear modulus for MOFs in the test set (GPa)

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**112.5**	**111.9**	**112.8**	**112.6**	**112.4**	**112.9**
PIJGEV (Cd)	**162.3**	**161.2**	**161.4**	**160.5**	**161.4**	**162.2**
HAWVOQ01 (Co)	**126.0**	**126.7**	**127.5**	**127.1**	**126.3**	**123.4**
QEJZUB01 (Cu I)	**149.4**	**147.8**	**147.5**	**149.3**	**148.0**	**149.2**
MURCEH (Cu II)	**172.1**	**171.2**	**170.2**	**171.9**	**173.1**	**176.0**
YORSII (Dy)	**137.9**	**137.6**	**137.6**	**137.0**	**138.1**	**141.3**
HOGWAB (Fe)	**136.8**	**127.1**	**127.4**	**129.0**	**127.0**	**132.9**
DEMLIR (Fe)	**144.5**	**144.3**	**143.1**	**144.8**	**144.8**	**142.6**
KOMJEC (Sm)	**155.8**	**155.1**	**155.1**	**153.2**	**154.3**	**160.0**
OFUWIV01 (Zn)	**157.0**	**156.7**	**156.6**	**156.5**	**157.7**	**156.1**

Table S 15: Minimum Poisson ration for MOFs in the test set

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**-1.16**	**-1.30**	**-1.25**	**-1.46**	**-1.43**	**-1.40**
PIJGEV (Cd)	**-0.35**	**-0.36**	**-0.35**	**-0.37**	**-0.35**	**-0.32**
HAWVOQ01 (Co)	**-0.79**	**-0.89**	**-0.82**	**-0.81**	**-0.82**	**-1.03**
QEJZUB01 (Cu I)	**-0.39**	**-0.50**	**-0.48**	**-0.54**	**-0.54**	**-0.39**
MURCEH (Cu II)	**-0.82**	**-0.81**	**-0.81**	**-0.82**	**-0.83**	**-0.85**
YORSII (Dy)	**-0.09**	**-0.09**	**-0.09**	**-0.09**	**-0.08**	**-0.06**
HOGWAB (Fe)	**-0.43**	**-0.39**	**-0.39**	**-0.43**	**-0.40**	**-0.31**
DEMLIR (Fe)	**0.02**	**0.03**	**-0.04**	**0.02**	**0.02**	**-0.02**
KOMJEC (Sm)	**-0.03**	**-0.03**	**-0.03**	**-0.04**	**-0.03**	**-0.03**
OFUWIV01 (Zn)	**-0.04**	**-0.05**	**-0.05**	**-0.04**	**-0.04**	**-0.06**

Table S 16: Maximum Poisson ration for MOFs in the test set

MOF	M06	PBE	PW91	PBE-D2	PBE-D3	vdw-DF2
RORQOE (Ag)	**1.70**	**1.83**	**1.78**	**2.01**	**1.97**	**1.94**
PIJGEV (Cd)	**0.78**	**0.79**	**0.78**	**0.78**	**0.78**	**0.77**
HAWVOQ01 (Co)	**1.74**	**2.04**	**1.84**	**1.85**	**1.88**	**2.18**
QEJZUB01 (Cu I)	**0.85**	**0.88**	**0.89**	**0.89**	**0.90**	**0.88**
MURCEH (Cu II)	**1.43**	**1.43**	**1.42**	**1.43**	**1.44**	**1.49**
YORSII (Dy)	**0.53**	**0.54**	**0.54**	**0.53**	**0.53**	**0.52**
HOGWAB (Fe)	**0.69**	**0.70**	**0.69**	**0.72**	**0.69**	**0.64**
DEMLIR (Fe)	**0.44**	**0.45**	**0.40**	**0.46**	**0.46**	**0.43**
KOMJEC (Sm)	**0.59**	**0.60**	**0.60**	**0.60**	**0.60**	**0.60**
OFUWIV01 (Zn)	**0.61**	**0.61**	**0.61**	**0.61**	**0.61**	**0.62**

Table S 17: The difference between MAD of vdw-DF2 and PBE-D2 for lattice parameters, bond lengths, Bond Angles and Torsion Angles. Negatives values are highlighted indicate that vdw-DF2 more accurately measured that property. Structures highlighted in red represent MOFs with little difference and highlighted in green represent MOFs with higher differences in predicted charges with vdw-DF2 and PBE and structures. We do not find a strong correlation between charge transfer predicted by vdw-DF2 and better prediction of structural parameters compared to PBE-D2.

	Lattice	Bond Length	Bond Angle	Torsion Angle
RORQOE (Ag)	-0.07	0.036	0.63	2.11
PIJGEV (Cd)	0.13	0.033	0.62	0.95
HAWVOQ01 (Co)	-0.12	0.017	2.11	6.21
QEJZUB01 (Cu I)	0.05	0.058	1.02	-0.09
MURCEH (Cu II)	0.12	0.026	-0.14	2.21
YORSII (Dy)	0.07	0.001	-1.29	2.28
HOGWAB (Fe II)	0.15	0.031	-0.2	-1.98
DEMLIR (Fe III)	-0.01	0.013	0.62	-0.60
KOMJEC (Sm)	-0.01	0.015	1.49	6.7
OFUWIV01 (Zn)	0.07	0.011	-0.88	2.14
GUPCUQ01 (Cd)	0.04	0.024	-0.43	-0.55

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