Supporting Information

Computational structure prediction of 4,4-connected copper paddle-wheel-based MOFs: Influence of ligand functionalization on the topological preference

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DFT Calculations

In this work, single-point energy calculations were performed at B3LYP/def-SV(P) level of theory. The resolution-of-identity (RI) approximation was used and the quadrature grid size was set at *m5*. In addition, D3 dispersion correction by Grimme was employed. The calculations were done by using the TURBOMOLE suite program (V7.1).

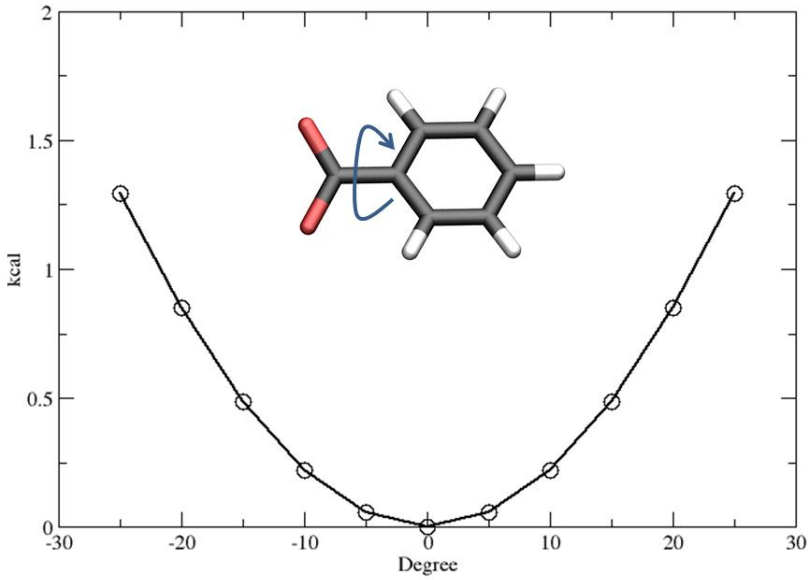

Figure S1. Energy profile for rotation of carboxylate plane (dihedral angle) in benzoate.

Table S1. Energy of the most stable structure of each topology in kcal/mol per f.u.

	nbo-b-L1	**ssa-L1**	**ssb-L1**	**lvt-b-L1**	**pts-L1**
vdW	12.77	10.76	11.11	10.48	8.49
Coulomb	-514.05	-512.81	-513.78	-512.60	-511.67
Non-bonding	**-501.29**	**-502.05**	**-502.68**	**-502.11**	**-503.18**
Stretching	2.24	2.22	2.13	2.25	2.68
Bending	27.66	28.46	27.98	28.43	29.69
Out-of-plane bending	0.31	2.87	0.22	2.75	4.29
Torsion	37.76	45.90	41.06	46.43	56.59
Bonding	**67.97**	**79.45**	**71.38**	**79.86**	**93.24**
TOTAL	**-433.32**	**-422.60**	**-431.29**	**-422.25**	**-409.95**
	nbo-b-L2	**ssa-L2**	**ssb-L2**	**lvt-b-L2**	**pts-L2**
vdW	9.48	10.27	7.98	8.35	8.54
Coulomb	-518.69	-517.20	-518.70	-517.26	-516.77
Non-bonding	**-509.21**	**-506.94**	**-510.72**	**-508.91**	**-508.22**
Stretching	2.73	2.82	2.90	2.75	3.45
Bending	27.13	27.80	27.28	27.73	29.19
Out-of-plane bending	0.34	2.68	0.56	2.83	5.07
Torsion	28.01	35.49	29.95	36.95	44.28
Bonding	**58.20**	**68.80**	**60.69**	**70.26**	**81.98**
TOTAL	**-451.01**	**-438.14**	**-450.03**	**-438.65**	**-426.25**
	nbo-b-L3	**ssa-L3**	**ssb-L3**	**lvt-b-L3**	**pts-L3**
vdW	10.22	21.31	7.41	9.59	9.23
Coulomb	-523.08	-520.06	-522.70	-521.68	-521.38
Non-bonding	**-512.86**	**-498.75**	**-515.29**	**-512.09**	**-512.15**
Stretching	2.81	5.06	2.98	2.87	4.04
Bending	27.62	32.95	28.18	28.33	30.95
Out-of-plane bending	0.32	2.45	0.39	2.86	5.32
Torsion	12.77	43.28	15.82	21.56	30.26
Bonding	**43.51**	**83.73**	**47.37**	**55.62**	**70.57**
TOTAL	**-469.35**	**-415.02**	**-467.92**	**-456.47**	**-441.58**