Supplemental information

Cooperative structural properties of a molecular motor functionalized Metal-Organic Framework: MotorMOF

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1. Force Field Parameterization

The force field parametrization is carried out following our reported parametrization protocol[1-5]. We extended the previously developed force field by using quantum mechanical (QM) reference data, calculated for a nonperiodic model of the organic motor functionalized linker (Fig. S1) at the density functional theory (DFT) level using the B3LYP+D functional[6, 7] and cc-pVDZ basis set[8] as implemented in Gaussian 16.[9] Analogous to our recently published *Motor-FF*[2], we defined new atom types for the core moiety of the motor and extended our *phoMOF-FF* parameter set,[1] which we previously parametrized using reference data at the same QM level, accordingly (see Fig. S1, blue marks atom-types of the standard MM3 FF and green/black marks new atom-types defining the core moiety of the molecular motor). The charges of the new atom-types are given by the Merz-Singh-Kollmann[10] charges of the reference system calculated on DFT level.

The parameter set describing the inorganic units is obtained from the *phoMOF-FF.* The parameters set for the inorganic unit together with the new parameter set of the organic motor functionalized linker establish the complete *MotorMOF-FF*. Note, the charges of atoms at connection points between organic and inorganic units or between motor moiety and *phoMOF-FF* atom-types are slightly modified for providing charge-neutrality of the organic building block and the complete MOF.

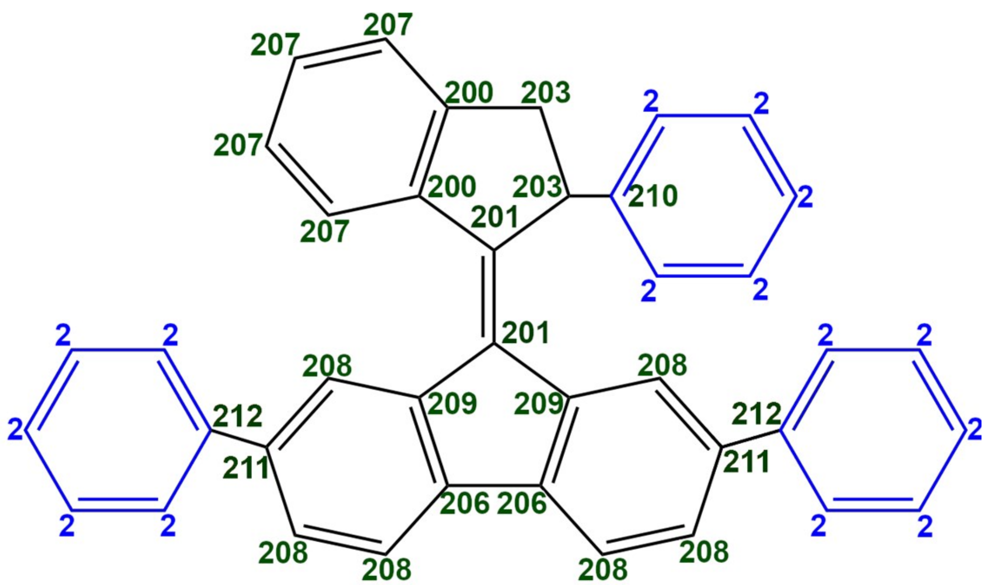


Figure S1: Scheme of the building block describing the motor functionalized linker. The green atom-types define the core moiety and blue describes obtained atom-types of the *phoMOF-FF*. The hydrogen (not shown) are represented by two atom-types 5 and 205. Atom-type 5 corresponds to the *phoMOF-FF* and atom-type 205 to the core moiety parameter set.

2. Force Field validation

a.

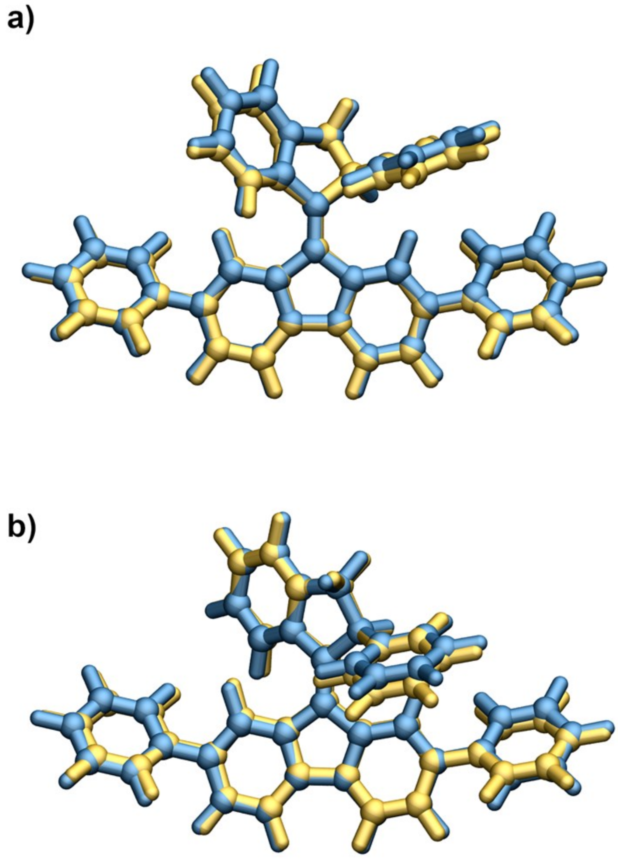


Figure S2. Overlay of the ball-and-stick model of the optimized building block structures in the stable (a) and meta-stable (b) state calculated at the DFT (blue) and with the *MotorMOF-FF* (orange) level.

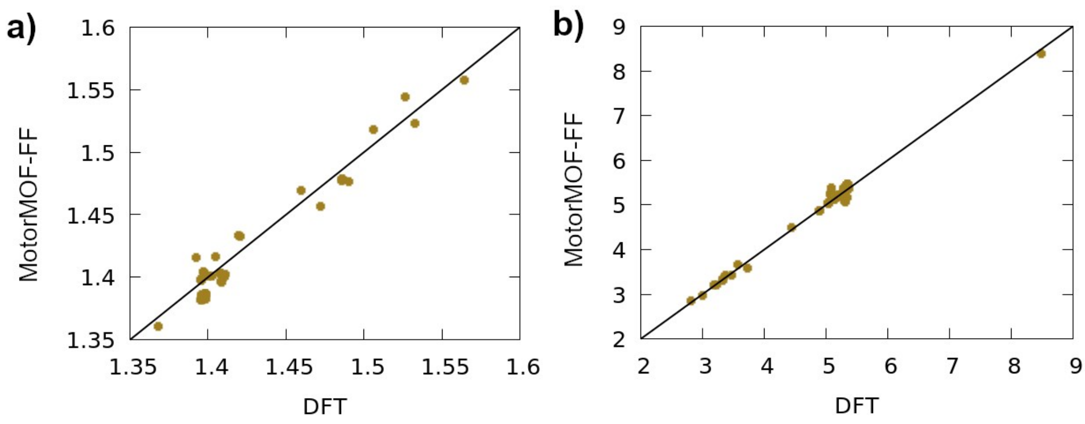


Figure S3. Comparison of the bond parameters of the motor-linker in stable state. The data were calculated at B3LYP+D3 level and using *MotorMOF-FF*. The bondlength of the optimized geometries are visualized in a) (in Å) and the corresponding force constants are given in b) (in mdyn/Å).

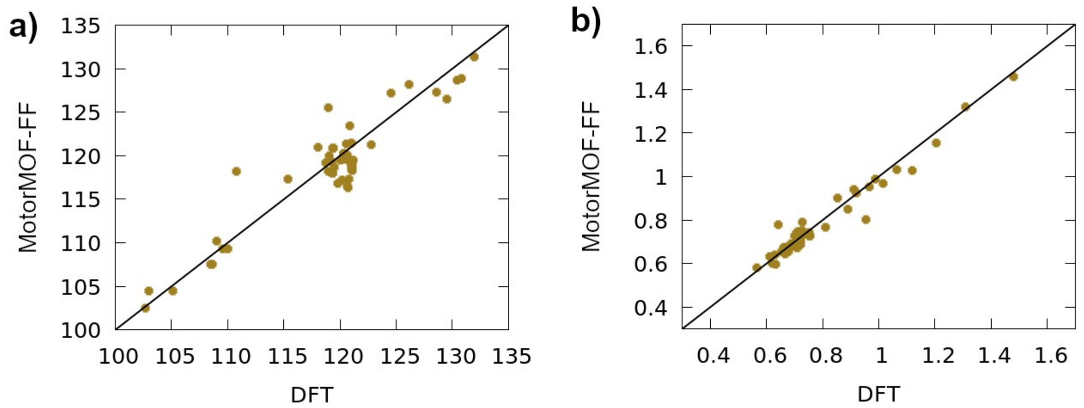


Figure S4. Comparison of the angle parameters of the motor-functionalized linker in stable state. The data were calculated on DFT level and using the FF approach. The angles of the optimized geometries are visualized in a) (in °) and the corresponding force constants are given in b) (in mdyn Å /rad^2).

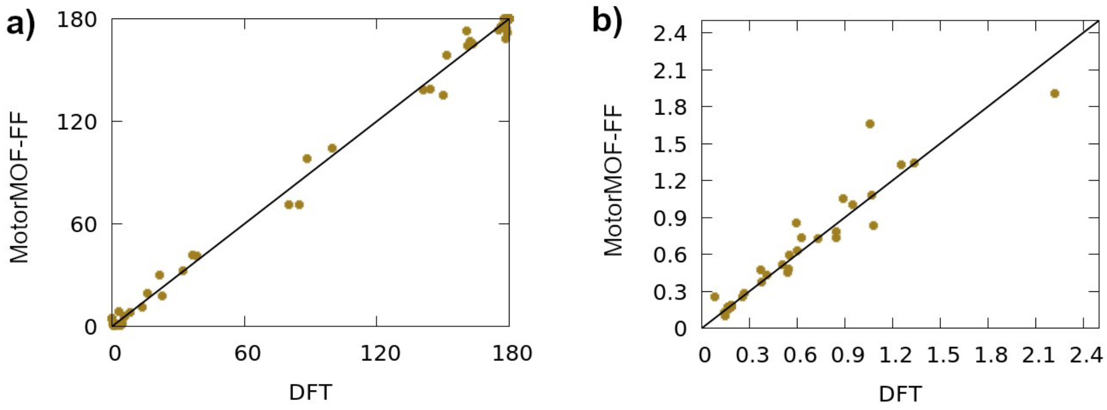


Figure S5. Comparison of the dihedral angle parameters of the motor-functionalized linker in stable state. The data were calculated on DFT level and using the FF approach. The dihedral angles of the optimized geometries are visualized in a) (in °) and the corresponding force constants are given in b) (in mdyn Å /rad^2).

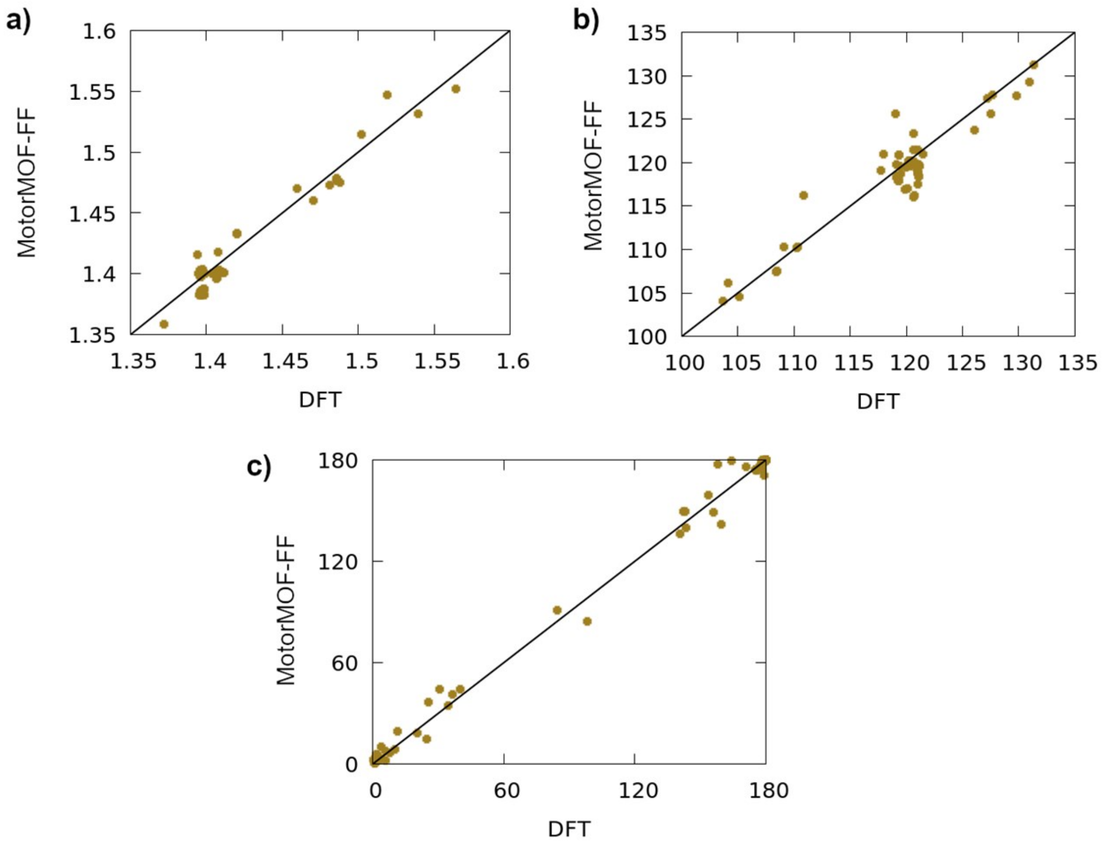


Figure S6. Bond length in Å (a), angles in degree (b), dihedral angles in degree (c) of the meta-stable motor functionalized linker calculated on DFT level and using the FF approach.

b. Normal mode analysis

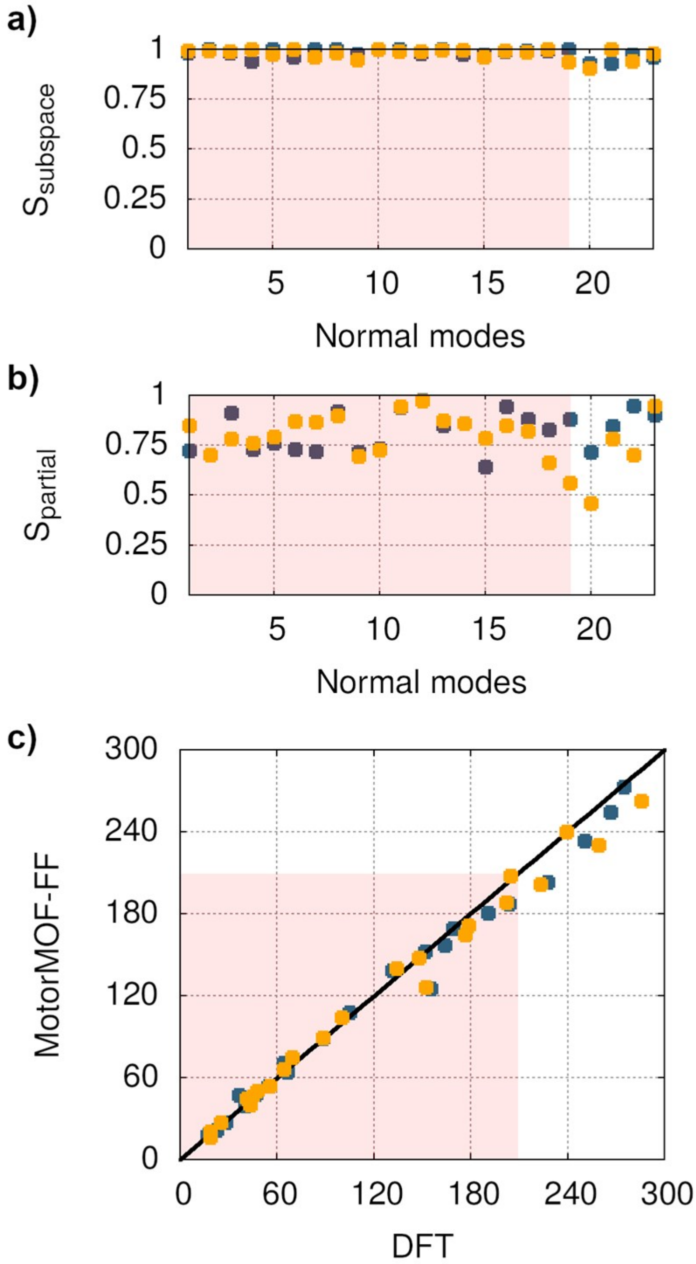


Figure S7: Comparison of the normal modes of the motor-functionalized linker in stable (blue) and meta-stable (orange) state. a) shows the projection of the DFT reference modes into the subspace of the *MotorMOF-FF* approach. b) shows the contribution of a single *MotorMOF-FF* mode with the highest agreement to a DFT mode. The x-axis in a) and b) counts the respective normal mode index of the reference system. c) illustrates a comparison of DFT and *MotorMOF-FF* eigenvalues. The red background marks the energy range up to 300 K.

3. Force Field Parameters

Table S1. Parameters for the bond stretch terms for the *MotorMOF-FF*

Bond stretch		k_b/mdyn/Å	r_b/Å
2	210	7.0682	1.3320
200	200	5.9640	1.4040
200	203	3.7400	1.5390
200	207	7.0730	1.4100
201	201	8.9700	1.3440
201	200	5.7050	1.4350
201	203	4.7491	1.4920
203	210	4.8374	1.5270
203	203	3.7355	1.5480
203	205	5.2450	1.0870
206	205	5.6550	1.1110
206	206	4.6560	1.4750
206	208	6.8630	1.3880
207	207	6.8910	1.3950
207	205	5.6960	1.0810
208	208	6.9660	1.3730
208	205	5.6720	1.0910
209	201	5.1360	1.4550
209	205	6.5600	1.0650
209	206	5.8270	1.4310
209	208	6.8324	1.3990
211	212	5.5190	1.4580
211	208	6.4840	1.3920
212	2	6.7680	1.3970
From *phoMOF-FF*:			
2	2	7.3460	1.3800
2	5	5.1500	1.1010
165	166	1.3300	1.9910
166	167	1.3300	1.9910
167	168	9.8260	1.2630
168	169	5.1400	1.1030
202	2	6.6360	1.4000
202	168	5.2380	1.4670

Table S2: Parameters for the in-plane angle bending terms for the *MotorMOF-FF*

In-plane angle bending			k_a/mdyn Å /rad^2	Θ_a/deg
2	210	2	0.7170	122.0000
2	212	211	1.0500	112.4860
2	212	2	0.6520	122.0000
200	200	203	0.5840	116.2700
200	203	205	0.7770	113.2590
200	207	205	1.0480	105.8430
200	207	207	1.5480	115.7070
201	203	210	0.8380	117.8670
201	209	205	1.8550	101.4340

201	209	206	1.8420	112.3290
201	209	208	1.0760	123.7100
201	201	200	0.7300	126.0000
201	201	203	0.7080	125.7230
201	201	205	0.8790	115.3760
201	200	200	1.1070	106.5430
201	200	205	0.1140	117.5520
201	203	203	1.2050	104.1170
201	203	205	0.8180	100.7590
203	210	2	0.6740	122.3000
203	203	210	0.9570	120.6530
203	201	200	0.8330	105.6440
203	200	205	1.2950	105.0670
203	203	200	0.7440	104.7460
203	203	205	0.6970	104.7450
205	203	205	0.5110	110.4650
206	209	205	1.7120	109.8890
206	209	208	0.4370	129.5460
206	206	205	1.7250	100.1540
206	206	208	1.0800	120.2060
206	208	205	0.8220	107.6410
206	208	208	1.1940	116.0070
207	200	201	0.5490	122.4110
207	200	200	0.5810	125.4820
207	200	203	0.9080	128.1550
207	207	205	0.9910	107.5310
207	207	207	1.1980	115.4900
208	208	205	0.7840	110.4980
208	208	208	0.9630	122.6260
208	211	212	1.4930	102.2000
208	211	208	1.3950	122.0000
209	201	209	0.5040	108.8850
209	201	201	1.3220	121.0550
209	201	205	0.5360	104.8620
209	206	205	0.7890	120.9040
209	206	206	0.5990	112.5580
209	206	208	0.8330	123.3960
209	208	205	0.7280	113.3470
209	208	208	0.9920	121.7410
210	2	5	0.4900	120.0000
210	2	2	0.8740	122.0000
210	203	205	0.5500	109.5000
211	208	208	0.8940	122.0000
211	208	209	1.0570	122.0000
211	208	205	0.4900	120.0000
212	2	5	0.4900	120.0000
212	2	2	0.8600	122.0000
From *phoMOF-FF*:				
2	2	2	0.7600	122.0000
2	2	5	0.4900	120.0000
2	202	2	0.7600	122.0000

2	202	168	0.8933	115.3120
165	166	167	0.2630	105.6000
166	165	166	0.0256	109.6370
166	167	168	0.1640	135.3400
167	168	167	1.1600	128.2760
167	166	167	0.2630	105.6000
167	168	202	1.1400	117.5230
202	2	2	0.9921	122.0000
202	2	5	0.4900	120.0000

Table S3: Parameters for the torsion terms for the extended *MotorMOF-FF*. The force parameters V_t^2 are in kcal/mol, dihedral angle τ_t^2 in degree and n defines the order of the fourier-term

torsion				V_t^2	τ_t^2	n	V_t^2	τ_t^2	n	V_t^2	τ_t^2	n	V_t^2	τ_t^2	n
2	212	211	208	0.0000	0.0	1	1.9000	180.0	2	0.0000	0.0	3	0	180	4
2	212	2	2	1.6940	0.0	1	4.2980	180.0	2	0.0000	0.0	3	0	180	4
2	212	2	5	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
2	210	2	2	4.7620	0.0	1	5.8370	180.0	2	0.0000	0.0	3	0	180	4
2	210	2	5	0.2500	0.0	1	9.0000	180.0	2	0.0000	0.0	3	0	180	4
200	201	201	209	9.0590	0.0	1	14.4810	180.0	2	2.8420	0.0	3	0	180	4
200	201	201	205	-0.7780	0.0	1	5.2720	180.0	2	0.0000	0.0	3	0	180	4
200	200	203	203	1.6040	0.0	1	9.9800	180.0	2	1.2030	0.0	3	0	180	4
200	200	203	205	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
200	200	207	205	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
200	200	207	207	2.2010	0.0	1	13.3320	180.0	2	4.7570	0.0	3	0	180	4
200	207	207	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
200	207	207	207	8.5070	0.0	1	1.6680	180.0	2	0.2640	0.0	3	0	180	4
201	209	206	208	1.1030	0.0	1	0.4180	180.0	2	0.4660	0.0	3	0	180	4
201	209	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
201	209	208	208	8.6160	0.0	1	-1.3240	180.0	2	0.9800	0.0	3	0	180	4
201	201	209	208	5.4350	0.0	1	4.5340	180.0	2	1.9700	0.0	3	0	180	4
201	201	200	200	-0.1270	0.0	1	5.2330	180.0	2	1.2650	0.0	3	0	180	4
201	200	200	203	-0.5260	0.0	1	11.3640	180.0	2	0.0000	0.0	3	0	180	4
201	200	200	205	0.0000	0.0	1	10.0000	180.0	2	0.0000	0.0	3	0	180	4
201	200	207	205	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
201	200	207	207	-1.4290	0.0	1	1.6890	180.0	2	7.5070	0.0	3	0	180	4
201	203	203	200	1.4100	0.0	1	16.1860	180.0	2	3.6240	0.0	3	0	180	4
201	203	203	205	0.0000	0.0	1	0.0000	180.0	2	0.5000	0.0	3	0	180	4
201	203	210	2	0.9470	0.0	1	2.1520	165.8	2	-0.7920	0.0	3	0	180	4
203	201	201	209	-2.4950	0.0	1	3.4050	180.0	2	1.6940	0.0	3	0	180	4
203	201	201	205	0.7730	0.0	1	13.7930	180.0	2	-1.0500	0.0	3	0	180	4
203	201	200	200	2.0410	0.0	1	1.9370	180.0	2	4.8710	0.0	3	0	180	4
203	200	200	207	-2.4330	0.0	1	-3.1580	180.0	2	0.0000	0.0	3	0	180	4
203	203	201	201	-0.1510	0.0	1	0.5780	180.0	2	0.7660	0.0	3	0	180	4
203	203	201	200	-2.1760	0.0	1	0.3500	180.0	2	-3.9640	0.0	3	0	180	4
203	210	2	5	0.0000	0.0	1	10.0000	180.0	2	0.0000	0.0	3	0	180	4
203	210	2	2	-2.9570	0.0	1	1.5490	180.0	2	0.0000	0.0	3	0	180	4
203	203	210	2	0.8210	0.0	1	0.3110	180.0	2	-1.7660	0.0	3	0	180	4

205	200	200	203	0.0000	0.0	1	10.0000	180.0	2	0.0000	0.0	3	0	180	4
205	200	200	205	0.0000	0.0	1	11.5000	180.0	2	0.0000	0.0	3	0	180	4
205	200	203	203	0.0000	0.0	1	0.0000	180.0	2	0.0100	0.0	3	0	180	4
205	200	203	205	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
205	203	201	201	0.0000	0.0	1	0.0000	180.0	2	-0.0900	0.0	3	0	180	4
205	203	201	200	0.0000	0.0	1	0.0000	180.0	2	-0.0900	0.0	3	0	180	4
205	203	203	200	0.0000	0.0	1	0.0000	180.0	2	0.5000	0.0	3	0	180	4
205	203	203	205	0.0000	0.0	1	0.0000	180.0	2	0.2380	0.0	3	0	180	4
205	207	200	200	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	207	200	203	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	207	207	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	207	207	207	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	208	208	209	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	208	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	208	208	206	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	208	208	208	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
205	208	211	208	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
205	203	210	2	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
206	209	201	209	1.7880	0.0	1	11.9660	180.0	2	0.8850	0.0	3	0	180	4
206	209	201	201	6.9680	0.0	1	3.7720	180.0	2	1.9180	0.0	3	0	180	4
206	209	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
206	209	208	208	1.5070	0.0	1	1.3800	180.0	2	0.5920	0.0	3	0	180	4
206	206	209	201	2.6140	0.0	1	7.2860	180.0	2	0.0370	0.0	3	0	180	4
206	206	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
206	206	208	208	-5.3760	0.0	1	0.8330	180.0	2	0.3530	0.0	3	0	180	4
206	208	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
206	208	208	208	-0.8260	0.0	1	5.9360	180.0	2	0.8300	0.0	3	0	180	4
207	200	201	201	3.3810	0.0	1	3.2860	180.0	2	3.7200	0.0	3	0	180	4
207	200	201	203	-2.4690	0.0	1	2.9420	180.0	2	0.3350	0.0	3	0	180	4
207	200	200	201	-0.2520	0.0	1	10.2920	180.0	2	0.0000	0.0	3	0	180	4
207	200	200	207	-5.1330	0.0	1	11.5900	180.0	2	0.0000	0.0	3	0	180	4
207	200	203	203	0.9540	0.0	1	6.8400	180.0	2	0.6160	0.0	3	0	180	4
207	200	203	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
207	207	200	200	0.5890	0.0	1	10.3650	180.0	2	0.5310	0.0	3	0	180	4
207	207	200	203	2.3240	0.0	1	3.0050	180.0	2	0.5930	0.0	3	0	180	4
207	207	207	205	3.1590	0.0	1	4.6390	180.0	2	0.0000	0.0	3	0	180	4
207	207	207	207	3.2390	0.0	1	2.6730	180.0	2	0.0000	0.0	3	0	180	4
207	207	207	207	0.5810	0.0	1	9.1790	180.0	2	0.0000	0.0	3	0	180	4
208	209	206	208	9.0430	0.0	1	3.3530	180.0	2	3.1420	0.0	3	0	180	4
208	209	206	206	4.7170	0.0	1	9.4870	180.0	2	0.5500	0.0	3	0	180	4
208	206	206	208	4.1110	0.0	1	-2.6390	180.0	2	1.1070	0.0	3	0	180	4
208	208	208	206	0.6280	0.0	1	3.2120	180.0	2	0.0000	0.0	3	0	180	4
208	208	208	208	5.9600	0.0	1	0.0270	180.0	2	0.0000	0.0	3	0	180	4
208	208	208	209	-0.3520	0.0	1	3.1900	180.0	2	0.0000	0.0	3	0	180	4
208	208	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
208	208	211	208	0.4060	0.0	1	22.8540	180.0	2	0.9240	0.0	3	0	180	4
209	201	209	208	2.1320	0.0	1	2.0490	180.0	2	1.9850	0.0	3	0	180	4
209	206	206	209	0.5070	0.0	1	7.1740	180.0	2	0.2430	0.0	3	0	180	4
209	206	206	208	-2.5030	0.0	1	8.8130	180.0	2	0.6090	0.0	3	0	180	4
209	206	208	205	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
209	206	208	208	-1.0390	0.0	1	18.0920	180.0	2	0.0130	0.0	3	0	180	4

209	208	208	205	0.2500	0.0	1	9.0000	180.0	2	-0.5500	0.0	3	0	180	4
209	208	208	208	-0.3050	0.0	1	2.1700	180.0	2	0.0000	0.0	3	0	180	4
209	208	211	208	1.0380	0.0	1	7.4220	180.0	2	0.4610	0.0	3	0	180	4
210	203	201	201	7.6000	0.0	1	4.1110	180.0	2	2.5200	0.0	3	0	180	4
210	203	201	200	-1.8770	0.0	1	-0.7270	180.0	2	-0.3630	0.0	3	0	180	4
210	203	203	200	-4.5500	0.0	1	-0.2880	180.0	2	1.1930	0.0	3	0	180	4
210	2	2	2	-4.8400	0.0	1	6.3310	180.0	2	0.3640	0.0	3	0	180	4
210	2	2	5	0.2500	0.0	1	9.0000	180.0	2	0.0000	0.0	3	0	180	4
210	203	203	205	0.0000	0.0	1	0.0000	180.0	2	0.5000	0.0	3	0	180	4
211	212	2	2	0.0410	0.0	1	5.5890	180.0	2	0.0000	0.0	3	0	180	4
211	212	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
211	208	209	201	1.7940	0.0	1	8.3280	180.0	2	0.0000	0.0	3	0	180	4
211	208	209	206	0.0510	0.0	1	6.3240	180.0	2	0.2960	0.0	3	0	180	4
211	208	208	206	0.9310	0.0	1	6.6230	180.0	2	3.7950	0.0	3	0	180	4
211	208	208	205	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
212	2	2	2	0.1560	0.0	1	11.1700	180.0	2	0.0030	0.0	3	0	180	4
212	211	208	208	4.0290	0.0	1	3.0660	180.0	2	0.0230	0.0	3	0	180	4
212	211	208	209	9.0510	0.0	1	10.3820	180.0	2	-3.8190	0.0	3	0	180	4
212	211	208	205	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
212	2	2	202	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
212	2	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
From *phoMOF-FF*:															
2	2	2	2	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
2	2	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
2	2	2	202	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
2	2	202	168	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
2	202	2	2	0.0000	0.0	1	5.9830	180.0	2	0.0000	0.0	3	0	180	4
2	202	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
5	2	2	5	0.0000	0.0	1	6.8810	180.0	2	0.0000	0.0	3	0	180	4
165	166	167	168	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
166	167	168	2	0.0000	0.0	1	0.0000	180.0	2	0.0000	0.0	3	0	180	4
166	165	166	167	0.0000	0.0	1	0.0000	180.0	2	0.0000	180.0	3	0	180	4
166	167	168	167	0.0000	0.0	1	4.1080	180.0	2	0.0000	0.0	3	0	180	4
166	167	168	169	0.7792	0.0	1	2.6942	180.0	2	0.6103	0.0	3	0	180	4
166	167	168	202	0.1130	0.0	1	3.1380	180.0	2	3.6880	0.0	3	0	180	4
167	166	167	168	0.0000	0.0	1	0.0000	0.0	2	0.0000	180.0	3	0	180	4
167	168	202	2	0.0000	0.0	1	4.6900	180.0	2	0.0000	0.0	3	0.198	180	4
168	202	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
168	202	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
202	2	2	5	0.0000	0.0	1	5.3850	180.0	2	0.0000	0.0	3	0	180	4
202	2	2	2	0.3820	0.0	1	9.5100	180.0	2	0.0000	0.0	3	0	180	4

Table S4. Parameters for the non-bonded terms of the M*otorMOF-FF*

Atom-type	radius 0.5 d_n^0/Å	ε_n/kcal/mol	bondlength reduction factor	charge
200	1.960	0.056		0.0661
201	1.960	0.056		-0.0536
203	2.040	0.027		-0.1158

205	1.620	0.020	0.923	0.1115
206	1.960	0.056		0.0285
207	1.960	0.056		-0.1409
208	1.960	0.056		-0.1682
209	1.960	0.056		0.0998
210	1.960	0.056		0.1635
211	1.960	0.056		-0.0227
212	1.960	0.056		-0.0227
from *phoMOF-FF*:				
2	1.960	0.056		-0.1200
5	1.620	0.020	0.923	0.1200
165	1.820	0.059		-1.4060
166	2.290	0.276		1.3040
167	1.820	0.059		-0.6610
168	1.940	0.056		0.8070
202	1.960	0.056		0.0000

Table S5. Parameters for the Out-of-plane terms of the *MotorMOF-FF*

Out-of-plane bending		Θ_0/deg	k_0/mdyn Å /rad^2
2	210	0.0000	0.2000
2	212	0.0000	0.0000
200	207	0.0000	0.0000
200	203	0.0000	0.0000
200	201	0.0000	0.0000
200	200	0.0000	0.0000
201	200	0.0000	0.0000
201	209	0.0000	0.0000
201	201	0.0000	0.0000
201	200	0.0000	0.0000
201	203	0.0000	0.0000
203	201	0.0000	0.0000
203	200	0.0000	0.0000
205	208	0.0000	0.0000
206	209	0.0000	0.0000
206	205	0.0000	0.0000
206	206	0.0000	0.0000
206	208	0.0000	0.0000
207	205	0.0000	0.0000
207	207	0.0000	0.0000
207	200	0.0000	0.0000
208	209	0.0000	0.0000
209	208	0.0000	0.0000
208	206	0.0000	0.0000
206	208	0.0000	0.0000
208	208	0.0000	0.0000
208	208	0.0000	0.0000
208	205	0.0000	0.0000

208	211	0.0000	0.0000
209	209	0.0000	0.0000
209	201	0.0000	0.0000
209	205	0.0000	0.0000
209	206	0.0000	0.0000
209	208	0.0000	0.0000
210	2	0.0000	0.2000
210	203	0.0000	0.1000
211	212	0.0000	1.2500
211	208	0.0000	0.0000
212	211	0.0000	1.2500
212	2	0.0000	0.0000
from *phoMOF-FF*:		0.0000	
2	2	0.0000	0.2000
2	5	0.0000	0.2000
2	202	0.0000	0.6013
168	167	0.0000	2.5000
168	202	0.0000	0.6485
202	2	0.0000	0.5084
202	168	0.0000	0.5643

Table S6: Parameters for the combined stretch-stretch and stretch-bend cross terms of the *MotorMOF-FF*

Combined stretch-stretch and stretch-bend cross terms			k_{sb1}/mdyn/rad	k_{s2}/mdyn/rad	k_{ss}/mdyn/Å
2	2	2	0.124	0.124	1.061
2	202	2	0.124	0.124	1.061
166	165	166	0.035	0.035	0.356
167	168	167	0.413	0.413	2.697
167	168	202	0.500	0.400	0.600
168	202	2	0.353	0.092	0.293

4. Genetic Algorithm

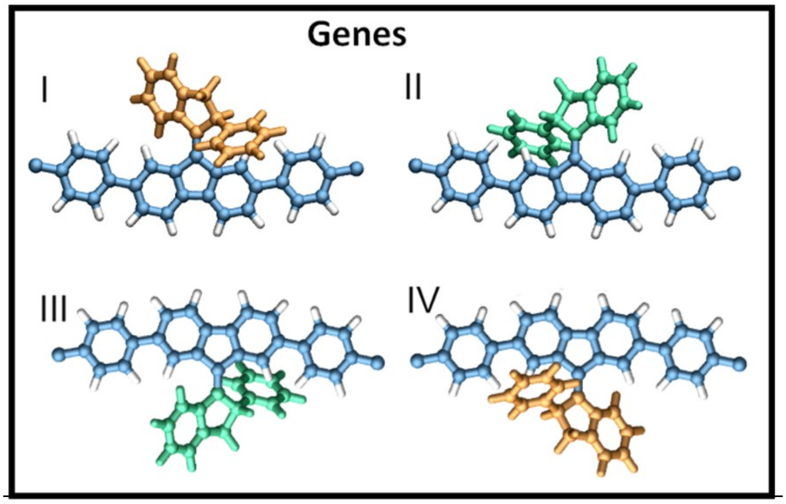
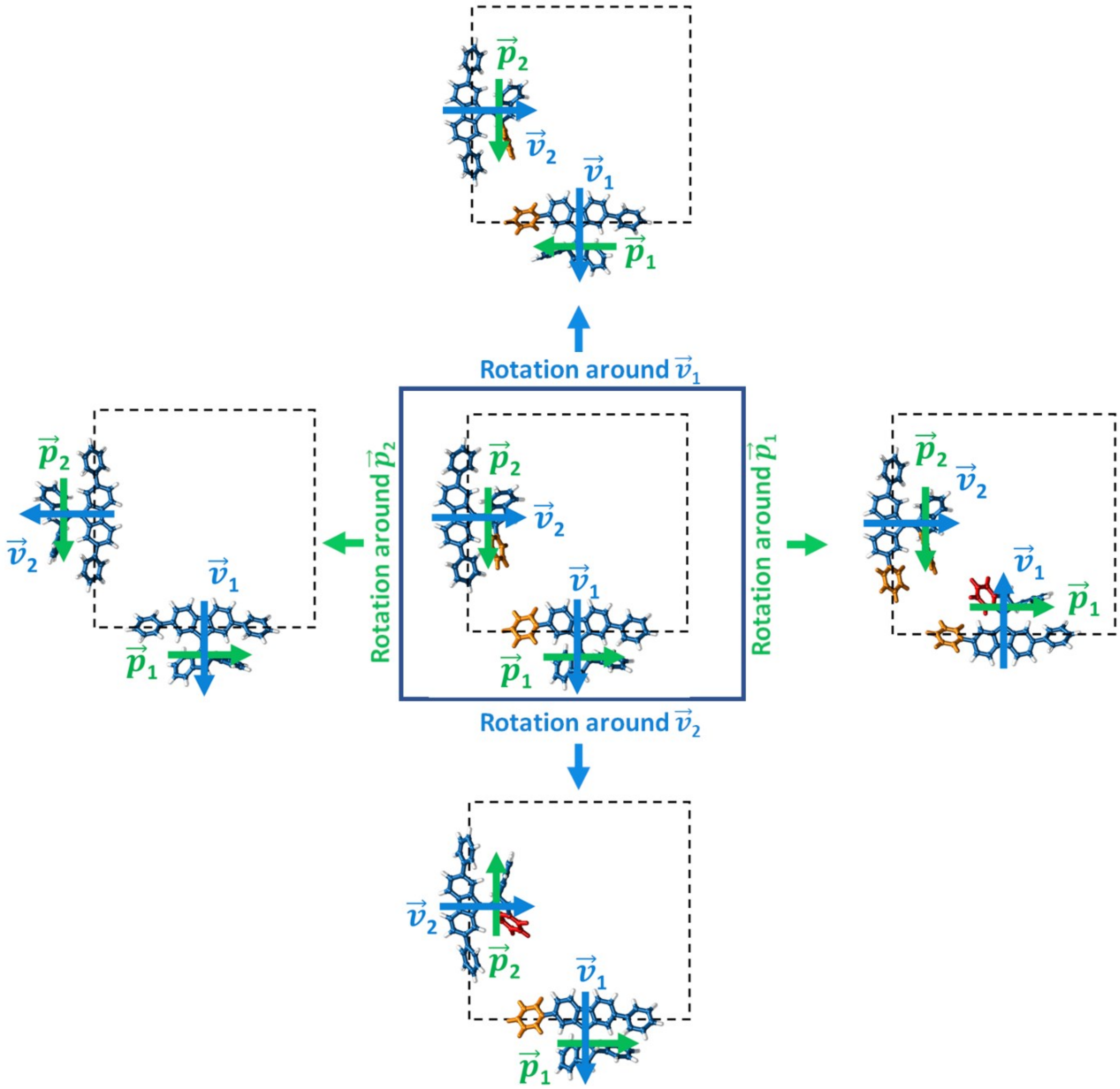


Figure S8. Four conformers of motor functionalized linker in meta-stable state, defining the possibilities of a gene for the GA.



5. Dimer Interaction

Figure S9. Visualization of the rotations around the characteristic vectors $\vec{v}_1$,$\vec{p}_1$,$\vec{v}_2$ and $\vec{p}_2$ starting from an initial dimer-structure (center image) a rectangular pattern. For rotations around $\vec{p}$ the rotation axis is placed along the grid. For simplicity only rotations around 180° are shown. The interaction ring-units are colored. Red indicates the benzene of the rotor, involved in the dimer interaction and orange involved phenyl-units.

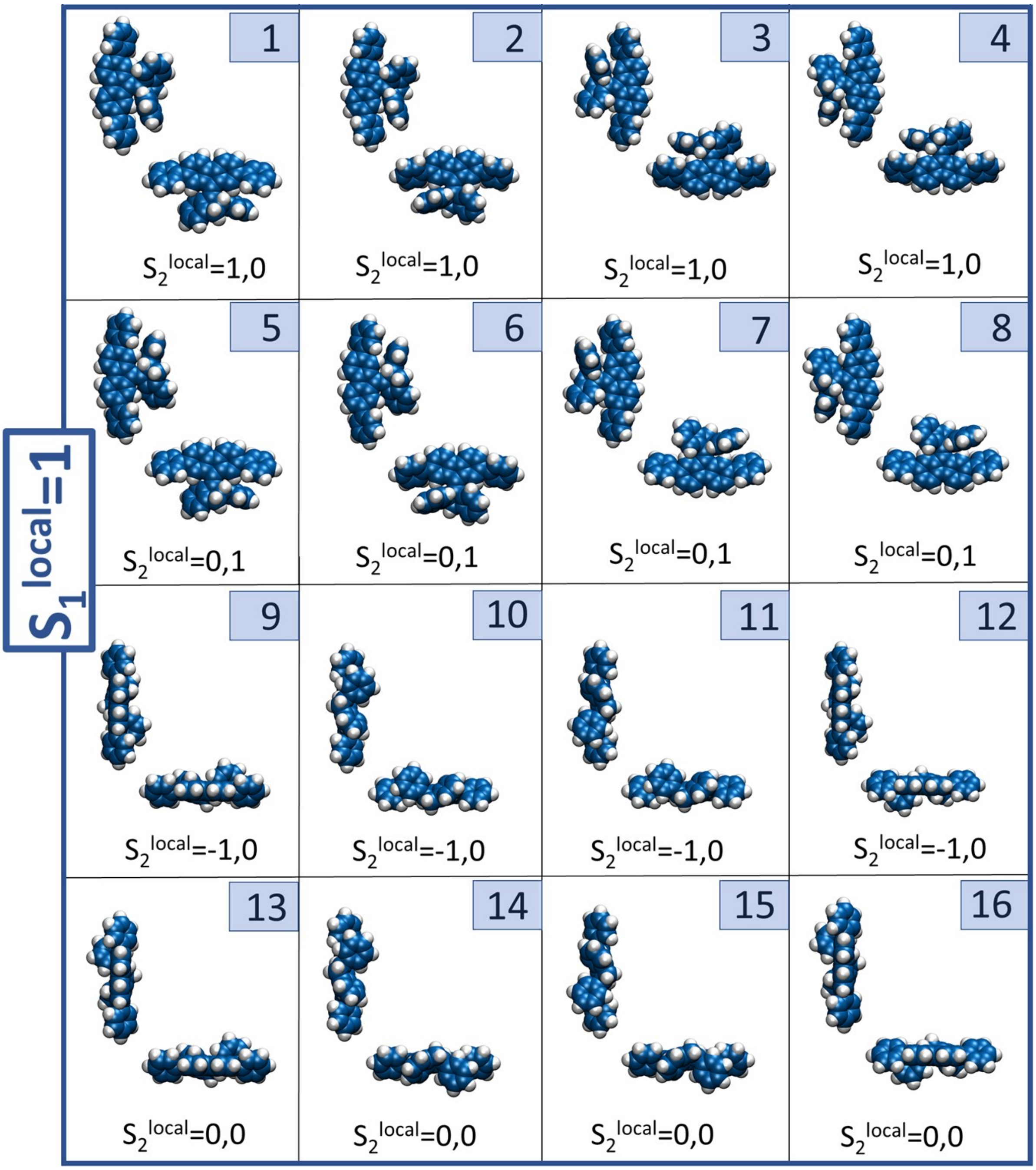


Figure S10. Visualization of all motor dimer-structures on a rectangular pattern with order parameter $S_1=1$. For simplicity only motors in stable state are shown.

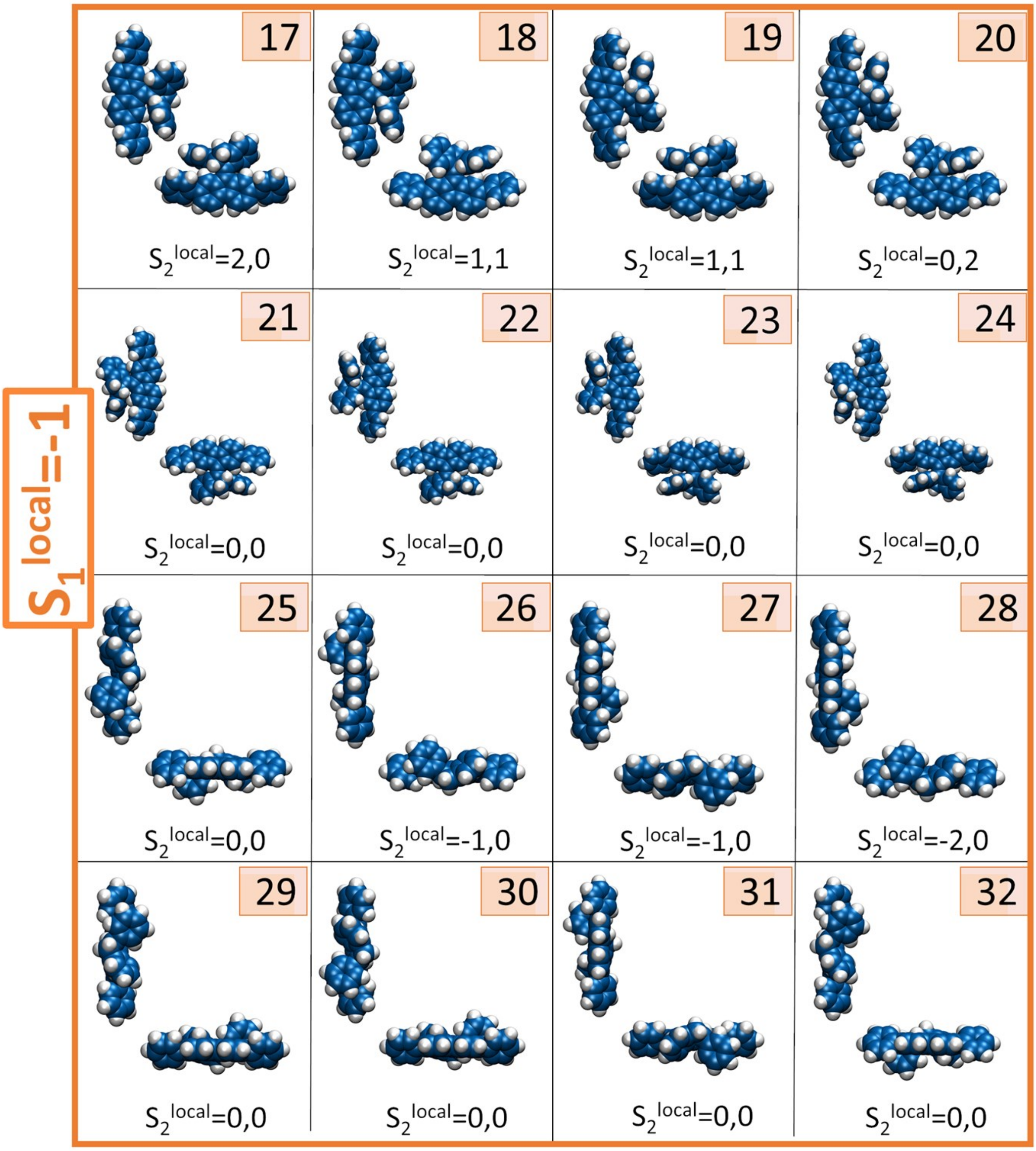


Figure S11. Visualization of all motor dimer-structures on a rectangular pattern with order parameter S_1=-*1*. For simplicity only motors in stable state are shown.

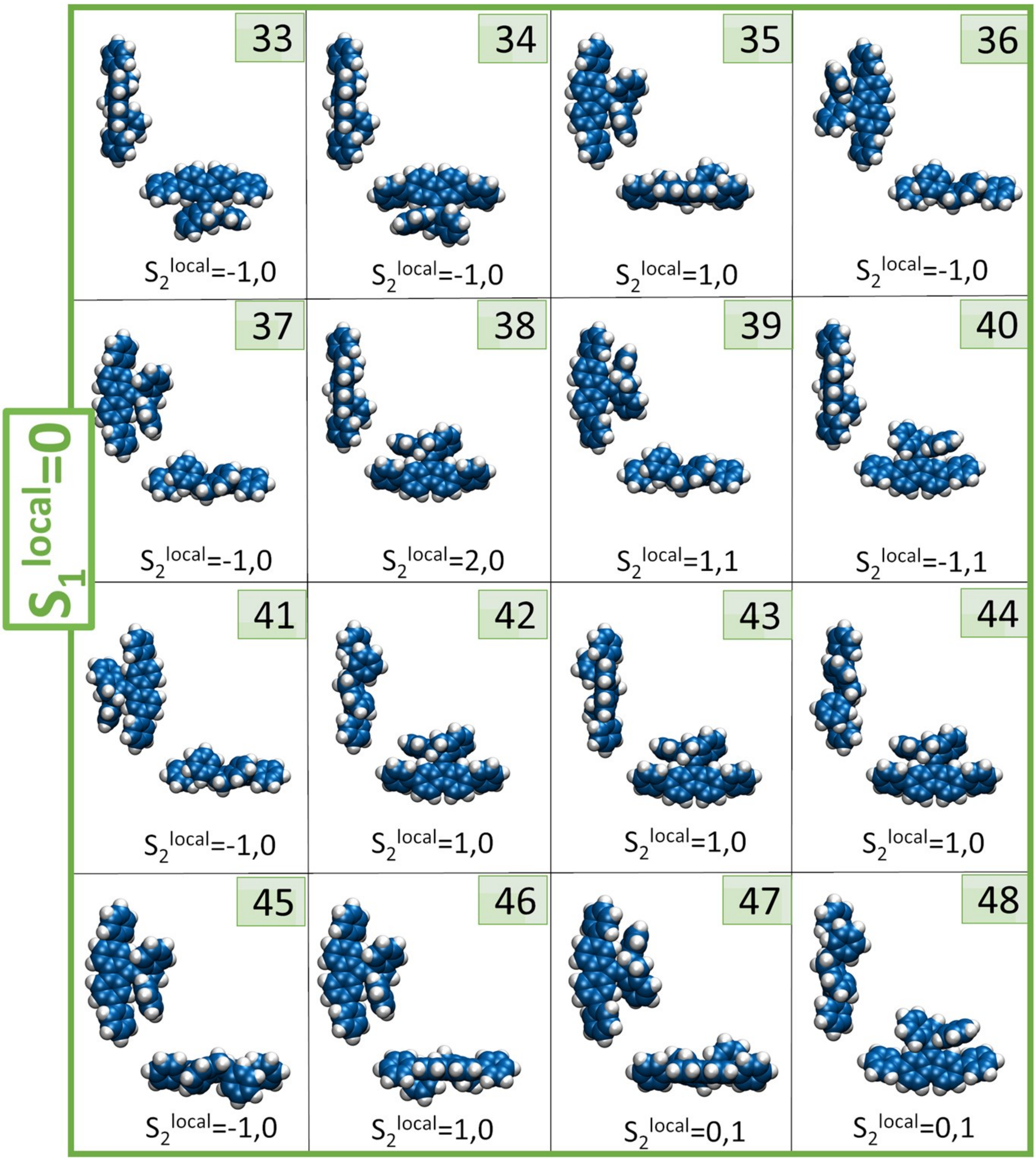


Figure S12. Visualization of half number of motor dimer-structures on a rectangular pattern with order parameter $S_1=0$. Remaining dimer-structures are shown in Figure S.13. For simplicity only motors in stable state are shown.

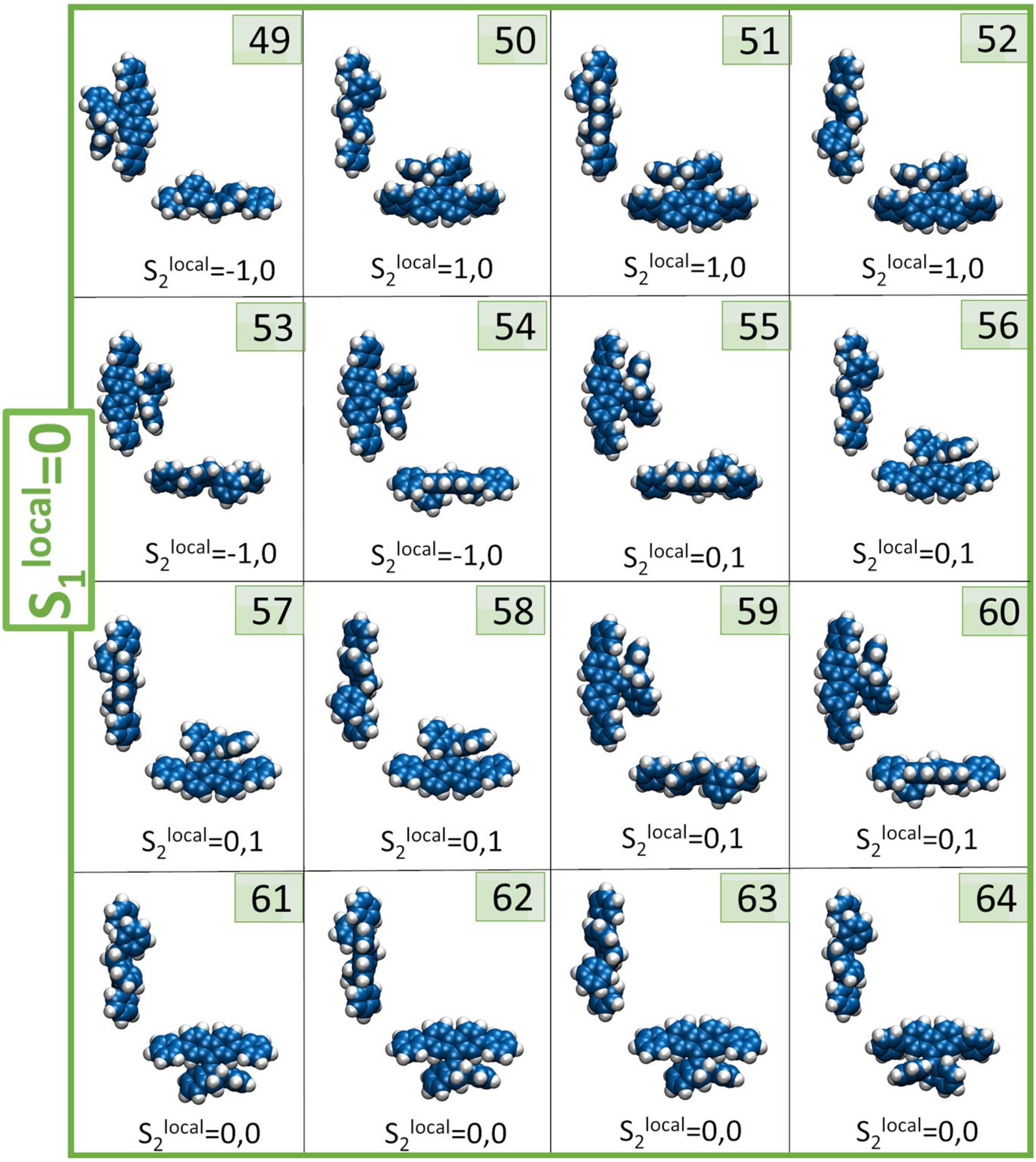


Figure S13. Visualization of half number of motor dimer-structures on a rectangular pattern with order parameter S_1=0. Remaining dimer-structures are shown in Figure S.12. For simplicity only motors in stable state are shown.

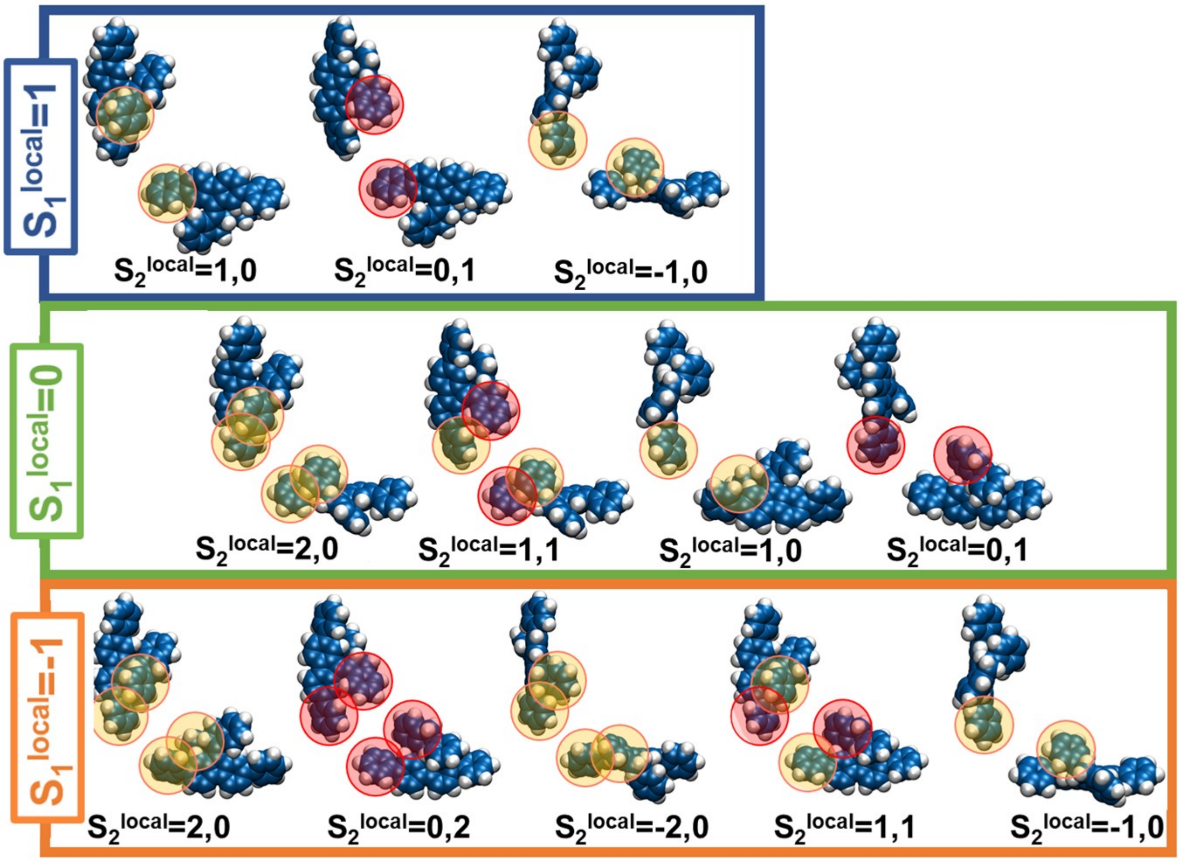


Figure S14. Visualization of different classes of interactions of motor functionalized linkers in meta-stable state on a rectangular pattern, representing the pore topology.

Table S1. Interaction energies in kcal/mol calculated on *MotorMOF-FF* and B3LYP+D level of dimers in different dimer classes of motor functionalized linkers in stable and meta-stable state. The orientated monomers are pre-optimized on MotorMOF-FF and B3LYP+D level respectively.

	stable		meta-stable	
	B3LYP+D	*MotorMOF-FF*	B3LYP+D	*MotorMOF-FF*
S_1=1	0.1 ± 0.1	0.2 ± 0.1	0.2 ± 0.1	0.2 ± 0.1
S_1=0	0.2 ± 0.1	0.2 ± 0.1	0.1 ± 0.1	0.1 ± 0.1
S_1=-1	0.2 ± 0.1	0.2 ± 0.1	0.1 ± 0.1	0.1 ± 0.1

6. Pore symmetry of an all-meta-stable cell

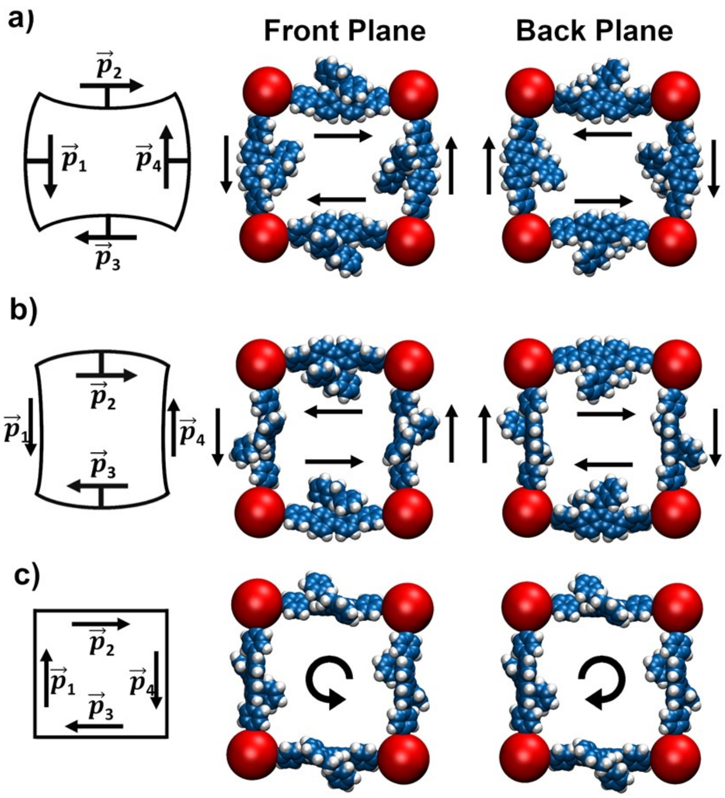


Figure S15. Van-der-Waals representation from a-direction (a), b-direction (b) and c-direction (c) of front and back plane of an **all-meta-stable** cell. The local ordering defined by $\vec{p}$ -vectors are visualized by black arrows

7. Definition of order parameters

For characterizing and quantifying the symmetry different order parameters are defined, describing local interactions (S7a), interactions over planes of the cubic MOF-structure (S7b) and global properties, describing the network in all three dimensions (S7c)

a. Local order parameter

The local order parameters S_1^{local} and S_2^{local} describe the relative orientation between two linkers aligned on a rectangular grid, which represents the pore topology, and allows thus a classification according to the order parameters. The order parameter S_1^{local} is defined by:

$$S_1^{local} = \vec{v}_i R_n \vec{v}_{i+1} \in [-1,1] \quad (1)$$

with $\vec{v}$ defined by the directions of the C=C double bond, pointing from the stator to the rotor part and subsequently projected onto the closest MOF plane.

The second order parameter S_2^{local} correlates the orientation of the ring-units of the respective rotor with relative arrangement of possible interaction partners. Therefore, S_2^{local} counts how many phenyl- and benzene-units of adjacent linkers are close enough for significant van der Waals interaction. In this regard a cut-off radius of 12 Å is introduced. For accomplishing the requirements, S_2^{local} is defined as a tuple of two values, where the first value counts the number of phenyl- and the second value counts the number benzene-interactions, which are within the cut-off radius. A minus sign indicates that the $\vec{v}$-vectors of both linkers are perpendicular to the rectangular plane.

This approach can be extended to analyze the geometry of a MotorMOF plane, by disassembling the layer into all possible pairs of linker-dimers. The order parameter S_1^{plane} is defined as the average of S_1^{local} over all linker-dimers

$$S_{1,j}^{plane} = \frac{1}{4}\frac{1}{n_c}\sum_{c}^{n_c}\sum_{i=1}^{4} S_{1,i,c}^{local} \quad \in [-1,1], \tag{2}$$

where the sum goes over all linker-dimers of the same plane around a corner (n_l) and further over all corners included in the used unit cell (n_c). In this way all linker-dimers corresponding to a MOF-plane are considered. Note, the used unit cell consists of two planes per crystallographic direction labeled with the variable *j*. Based on this, the plane order parameters are calculated by

$$S_{1}^{plane} = \frac{1}{2}\sum_{j=1}^{2} S_{1,j}^{plane} \quad \in [-1,1]. \tag{3}$$

The corresponding order parameter S_2^{plane} is given by the distribution of occurring interaction types visualized in Fig. 3c).

b. Global correlation parameter

The global correlation parameter S_1^{global} is defined to evaluate correlation and ordering within a three-dimensional MotorMOF system. Here, the energetically most preferred MotorMOF structure is used as reference to calculate the correlation parameter S_1^{global}, which considers the symmetry of the a-plane described by $S_1^{plane,a}$ with respect to the perpendicular b-plane. Based on this, all dimers within the a-plane and all linker perpendicular are considered and correlated. The ordering between linkers of the a-plane and the b-plane is thus calculated by

$$S^{corr-a,b}_{1,j} = \frac{1}{4n_c}\sum_{c}^{n_c}\sum_{i}^{4}\left(\vec{v}_i \times \vec{v}_{i+1}\right) \cdot \vec{e}_n \in [-1,1], \qquad (4)$$

where $\vec{e}_n$ is the normal vector of the MOF-plane perpendicular to the crystallographic b-direction and j numbers the respective layer within the unit cell.

The total correlation parameter is therefore defined by

$$S^{corr-a,b}_{1} = \frac{1}{2}\left|\sum_{j=1}^{2} S^{corr-a,b}_{1,j}\right| \in [0,1] \qquad (5)$$

where j counts the planes per crystallographic direction, and according to these definitions follows:

$$S^{global}_{1} = \frac{1}{2}\left(S^{plane,a}_{1} + S^{corr-a,b}_{1}\right) \in [-1,1]. \qquad (6)$$

The global correlation parameter S_1^{global} describes the linkers arrangement along the a-plane by $S_1^{plane-a}$ and considers at the same time the remaining linkers perpendicular to that by $S_{1,j}^{corr-a,b}$.

Note, equation (4) is strongly related to equation (2) describing the symmetry of the b-plane by $S_{1,j}^{plane-b}$, but it is modified by the cross product. This modification results in a maximized global correlation parameter $S_1^{global}=1$ for the energetically preferred pore topology of the MotorMOF. By applying this formalism on other MotorMOFs with different linker configurations, a value of $S_1^{global}=1$ indicates the same pore topology in all three crystallographic directions with respect to the energetically preferred MotorMOF. Whereas a value of $S_1^{global}=0$ implies that the topology of the compared structure differs significantly from the predesign energetically lowest MOF topology. The definition of equation (4) thus enables to compare the overall pore topology of different MotorMOFs und thus quantify structural correlations.

Since the order parameter S_1^{global} only considers the direction of the rotor with respect to the stator ($\vec{v}$) and thus the curvature of the MOF scaffold, a second global correlation parameter S_p^{global}, is introduced to take into account the local pore symmetry. The global correlation parameter S_p^{global}, describes the relative orientation of neighboring rotors $\vec{p}$ by a local pore order parameter S_p^{local}, which is defined analogous to equation (1) by

$$S_p^{local} = \vec{p}_i R_n \vec{p}_{i+1} \in [-1,1]. \quad (7)$$

where the rotation matrix R_n rotates a linker of the pore anticlockwise along the pore plane on its neighbor. The global order parameter S_p^{global} is defined as the average over the plane-related order parameters S_p^{plane} given by

$$S_{p,j}^{plane} = \frac{1}{n_c}\frac{1}{n_l}\sum_{c}^{n_c}\sum_{i=1}^{4} S_{p,i,c}^{local} \cdot f(plane) \in [-1,1]. \quad (8)$$

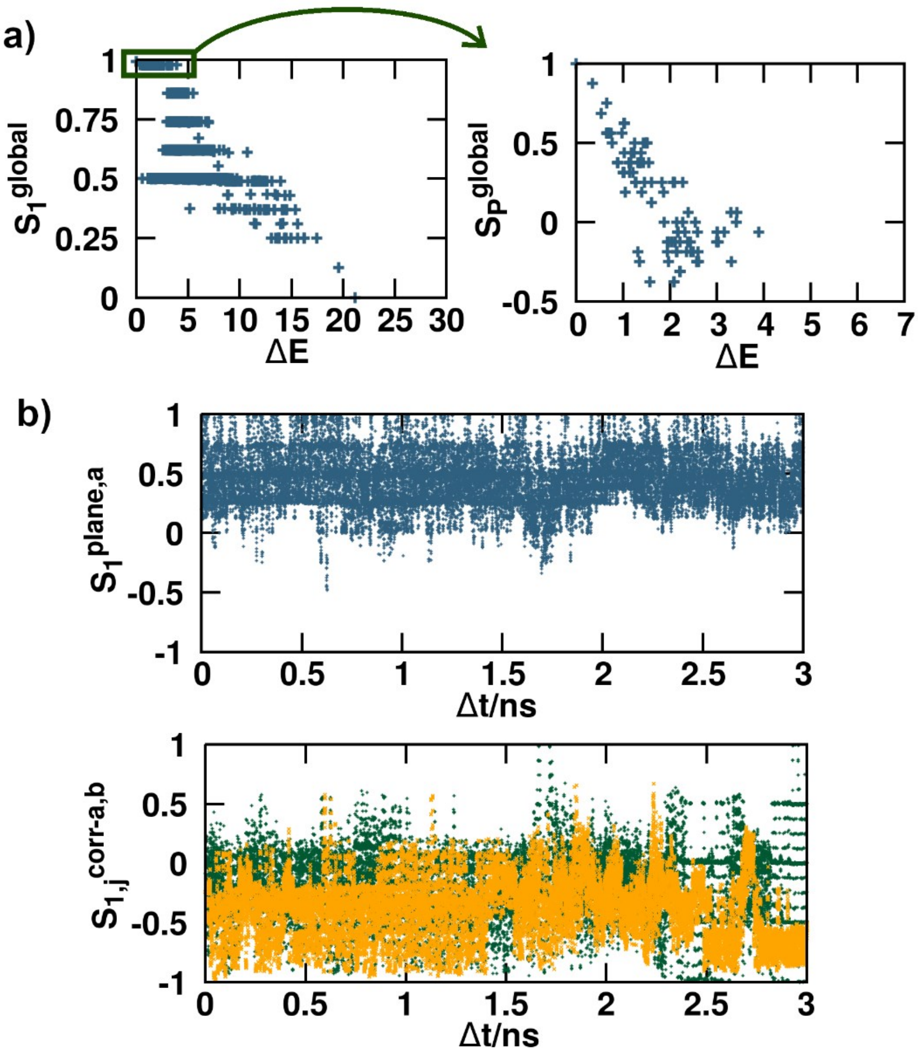
Considering both layers within the unit cell S_p^{plane} is

$$S_p^{plane} = \frac{1}{2}\sum_{j=1}^{2} S_{p,j}^{plane} \in [-1,1]. \quad (9)$$

For describing all linkers with respect to each other, two planes must be involved for the S_p^{global} calculation:

$$S_p^{global} = \frac{1}{2}\left(S_p^{plane,a} + S_p^{plane,b}\right) \in [-1,1]. \quad (10)$$

Using the sign-function, the pore symmetry of the energetically preferred MotorMOF, depicted in Fig. 4 for **all-stable** and in Fig. S10 for **all-meta-stable** MotorMOF, gives a value of 1 for S_p^{global}.



8. Global ordering of all-meta-stable MOFs

Figure S16. a) Order parameter S_1^{global} and S_P^{global} indicating local and global linker arrangement of the **all-stable** MOF. b) visualizes different possible rotations of the linker during the GA construction and MD simulations. c) Order parameter $S_1^{plane-a}$ during a MD simulation, as well as its coupled correlation parameters $S_{1,1}^{corr-a,b}$ (orange) and $S_{1,2}^{corr-a,b}$ (green) of the **all-meta-stable** MOF, describing the correlation between the both planes in the unit cell, which are perpendicular to the a-direction and both planes perpendicular to the b-direction.

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