Supporting Information

Computational screening of metal-organic framework structures for separation of propane/propene mixture

Viral A. Solanki and Bhaskarjyoti Borah*

P. D. Patel Institute of Applied Sciences, Charotar University of Science & Technology,

Changa, Anand, Gujarat – 388421, India

E-mail: bhaskarborah.phys@charusat.ac.in

1. Potential Parameters

Table S1 Lennard-Jones potential parameters for various atoms of the MOFs

Atom Type	ϵ/k_B[K]	σ [Å]
Ac	16.6	3.1
Ag	18.11	2.8
Al	254.09	4.01
Am	7.04	3.01
Ar	93.08	3.45
As	155.47	3.77
At	142.89	4.23
Au	19.62	2.93
B	90.57	3.64
Ba	183.15	3.3
Be	42.77	2.45
Bi	260.63	3.89
Bk	6.54	2.97
Br	126.29	3.73
C	52.83	3.43
Ca	119.75	3.03
Ca	119.75	3.03
Cd	114.72	2.54
Ce	6.54	3.17
Cf	6.54	2.95
Cl	114.21	3.52
Cm	6.54	2.96
Co	7.04	2.56
Cr	7.55	2.69
Cu	2.52	3.11
Cs	22.64	4.02
Dy	3.52	3.05
Eu	4.03	3.11
Er	3.52	3.02
Es	6.04	2.94
F	25.16	3
Fe	6.54	2.59
Fm	6.04	2.93
Fr	25.16	4.37
Ga	208.81	3.9
Ge	190.69	3.81
Gd	4.53	3

H	22.14	2.57
Hf	36.23	2.8
Hg	193.71	2.41
Ho	3.52	3.04
I	170.57	4.01
In	301.39	3.98
Ir	36.73	2.53
K	17.61	3.4
Kr	110.69	3.69
La	8.55	3.14
Li	12.58	2.18
Lu	20.63	3.24
Lr	5.53	2.88
Md	5.53	2.92
Mg	55.85	2.69
Mn	6.54	2.64
Mo	28.18	2.72
N	34.72	3.26
Na	15.09	2.66
Ne	21.13	2.66
Nb	29.69	2.82
Nd	5.03	3.18
No	5.53	2.89
Ni	7.55	2.52
Np	9.56	3.05
O	30.19	3.12
Os	18.62	2.78
P	153.46	3.69
Pa	11.07	3.05
Pb	333.59	3.83
Pd	24.15	2.58
Pm	4.53	3.16
Po	163.52	4.2
Pr	5.03	3.21
Pt	40.25	2.45
Pu	8.05	3.05
Ra	203.27	3.28
Rb	20.13	3.67
Re	33.21	2.63
Rh	26.67	2.61
Rn	124.78	4.25
Ru	28.18	2.64
S	137.86	3.59

Sb	225.91	3.94
Sc	9.56	2.94
Se	146.42	3.75
Si	202.27	3.83
Sm	4.03	3.14
Sn	285.28	3.91
Sr	118.24	3.24
Ta	40.75	2.82
Tb	3.52	3.07
Tc	24.15	2.67
Te	200.25	3.98
Th	13.08	3.03
Ti	8.55	2.83
Tl	342.14	3.87
Tm	3.02	3.01
U	11.07	3.02
V	8.05	2.8
W	33.71	2.73
Xe	167.04	3.92
Y	36.23	2.98
Yb	114.72	2.99
Zn	62.39	2.46
Zr	34.72	2.78

a. Force field for propene

Non-bonded LJ parameters for propene

Atom ID	Pseudo atom	Atom type	ϵ/k_B (K)	σ (Å)
1	CH3	$[CH_3]$-CH_x	98	3.75
2	CH	CH_x=[CH]-CH_y	47	3.73
3	CH2	$[CH_2]$==CH_x	85	3.675

Intramolecular potential parameters for propene

Bond ID	Stretch	Type	Length (Å)
1	1 – 2	CH_x-CH_y	1.54
2	2 – 3	CH_x=CH_y	1.33

The bond angle bending is modelled with the following harmonic function

$$U_{bend} = \frac{k_\theta}{2}(\theta - \theta_0)^2$$

Angle ID	Bend	Type	θ_0 (in degrees)	k_θ/k_B (K/rad^2)
1	1 – 2 – 3	CH_x=(CH)-CH_x	119.70	70420

b. Force field for propane

Non-bonded LJ potential parameters for propane

Atom ID	Pseudo atom	Atom type	ϵ/k_B (K)	σ (Å)
1	CH_3	CH_3-CH_x	98	3.75
2	CH_2	CH_x-CH_2-CH_x	46	3.95
3	CH_3	CH_3-CH_x	98	3.75

Intramolecular potential parameters for propane

Bond ID	Stretch	Type	Length
1	1 – 2	CH_x-CH_y	1.54
2	2 – 3	CH_x-CH_y	1.54

The bond angle bending in propane is modelled using the following harmonic function

$$U_{bend} = \frac{k_\theta}{2}(\theta - \theta_0)^2$$

Angle ID	Bend	Type	θ_0 (in degrees)	k_θ/k_B (K/rad^2)
1	1 – 2 – 3	CH_x-(CH_2)-CH_y	114	62500

2. Correlations of all the structural properties of the MOFs

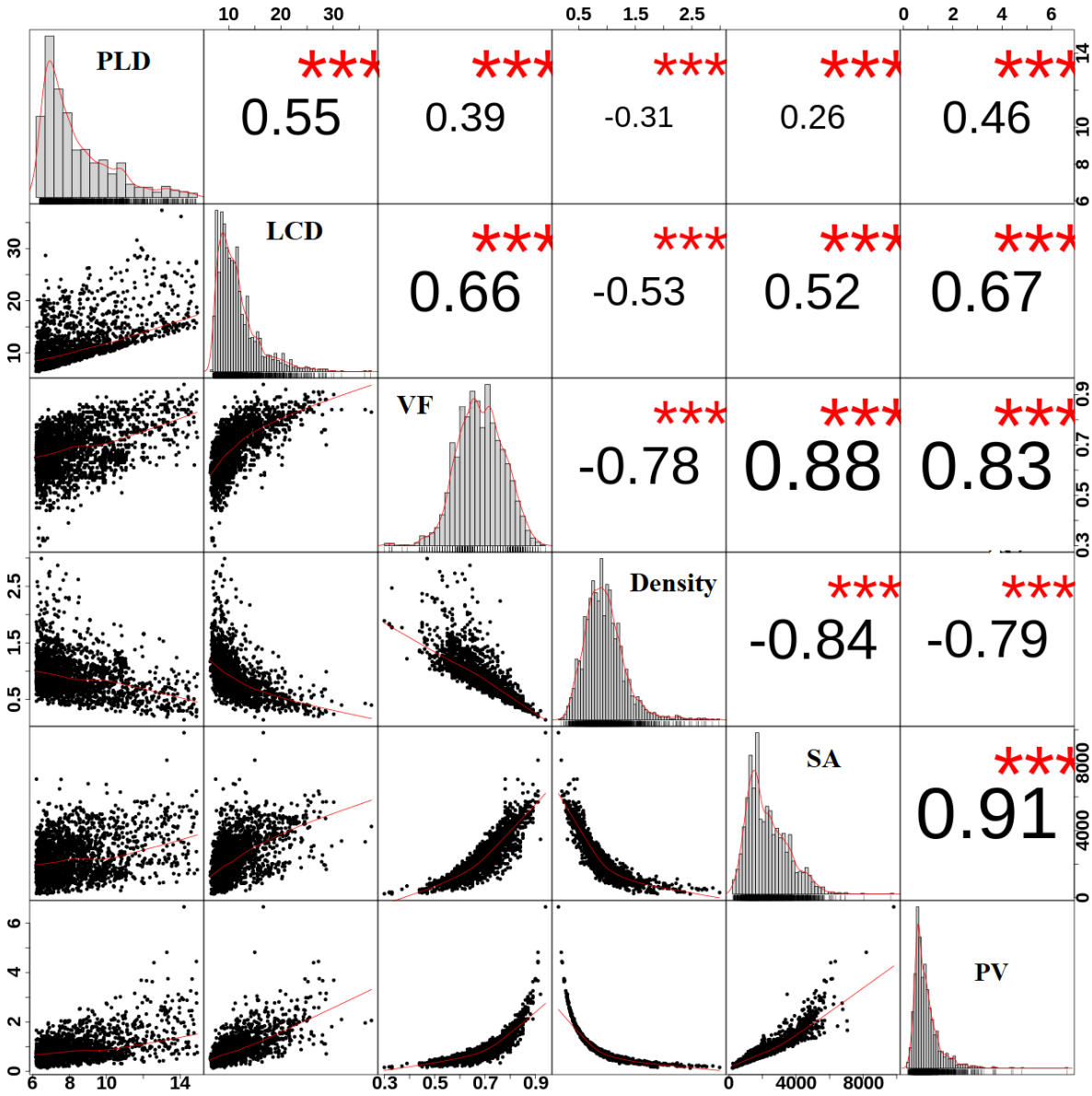

Figure S1 Correlations of all the structural properties of the MOFs. Each point corresponds to one MOF structure, the red lines are guides to the eye showing the trend line. The numbers in the boxes indicate the correlation coefficients and the stars indicate the significance level of the correlations. Three stars indicate p-value is 0.001; two stars indicate p-value is 0.01 and single star indicate p-value is 0.05.

3. Regenerability as functions of structural properties

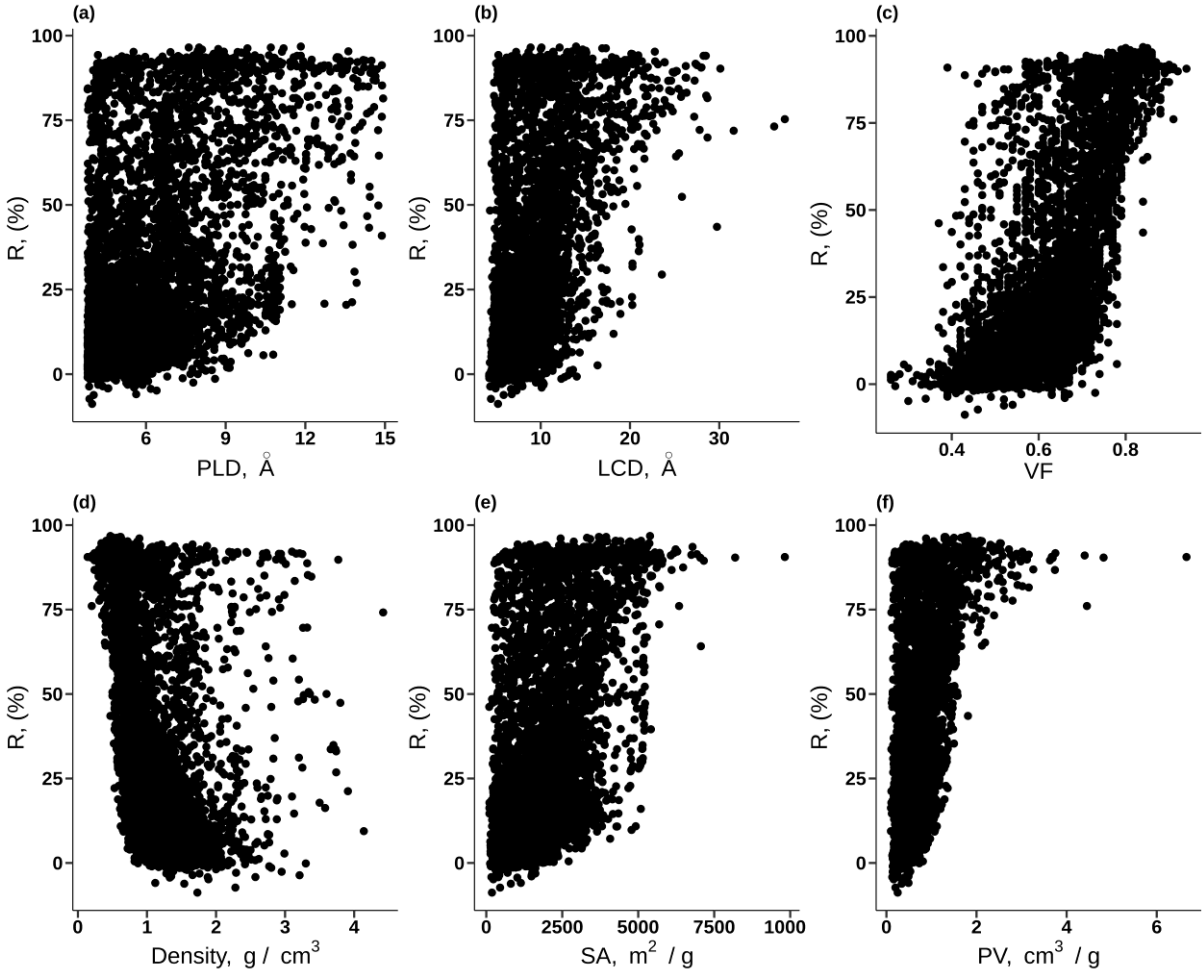

Figure S2 Regenerability plotted as functions of (a) PLD (b) LC (c) void fraction (VF) (d) Density (e) Surface area (SA) (f) pore volume (PV). Each point corresponds to one MOF structure.

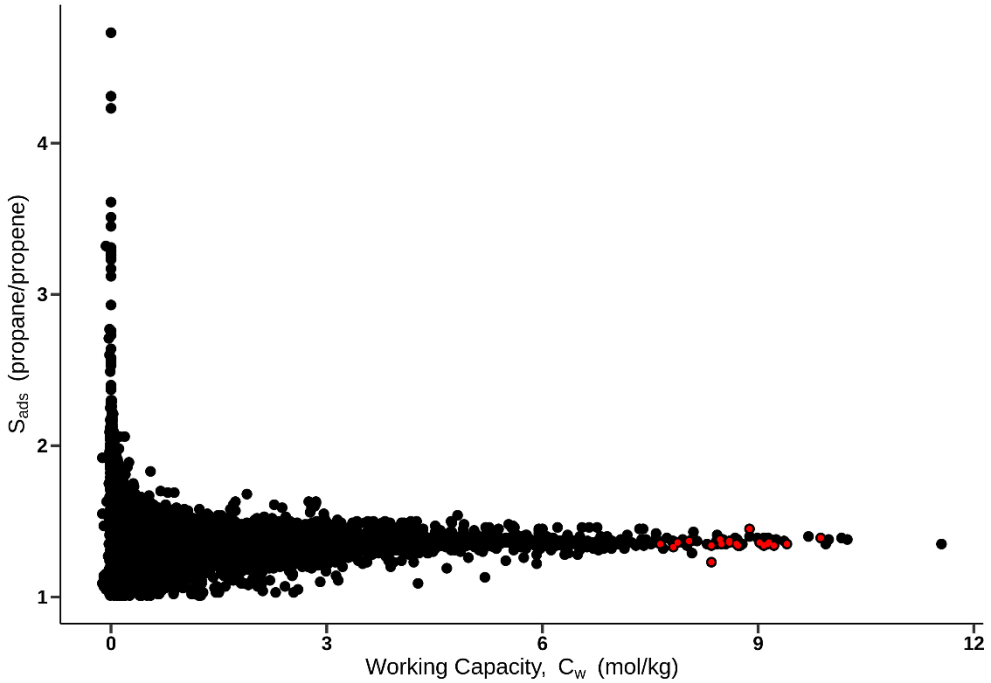

Figure S3 Adsorption selectivity as a function of working capacity showing the trade-off between these two quantities. Each point corresponds to one MOF structure. The red points indicate the top performing MOFs.