Supporting Information: High-throughput assessment of hypothetical zeolite materials for their synthesizeability and industrial deployability

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SI1 Zeolite Lists

SI1.1 IZA Frameworks Used in This Work

ABW	ACO	AEI	AEL	AEN	AET	AFG
AFI	AFN	AFO	AFR	AFS	AFT	AFV
AFX	AFY	AHT	ANA	APC	APD	AST
ASV	ATN	ATO	ATS	ATT	ATV	AVL
AWO	AWW	BCT	BEA	BEC	BIK	BOF
BOG	BOZ	BPH	BRE	BSV	CAN	CAS
CDO	CFI	CGF	CGS	CHA	CON	CSV
CZP	DAC	DDR	DFO	DFT	DOH	DON
EAB	EDI	EEI	EMT	EON	EPI	ERI
ESV	ETR	EUO	EZT	FAR	FAU	FER
FRA	GIS	GIU	GME	GON	GOO	HEU
IFO	IFR	IFW	IFY	IHW	IMF	IRN
IRR	ISV	ITE	ITG	ITH	ITR	ITT
ITW	IWR	IWS	IWV	IWW	JBW	JNT
JOZ	JRY	JSN	JSR	JST	JSW	KFI
LAU	LEV	LIO	LOS	LOV	LTA	LTF
LTJ	LTL	LTN	MAR	MAZ	MEI	MEL
MEP	MER	MFI	MFS	MON	MOR	MOZ
MRE	MSE	MSO	MTF	MTN	MTT	MTW
MVY	MWW	NAB	NAT	NES	NON	NPO
NPT	NSI	OBW	OFF	OKO	OSI	OSO
OWE	PAU	PCR	PHI	PON	POS	PSI
PUN	RHO	RRO	RSN	RTE	RTH	RUT
RWR	SAF	SAO	SAS	SAT	SAV	SBE
SBN	SBS	SBT	SEW	SFE	SFF	SFG
SFH	SFN	SFO	SFS	SFW	SGT	SIV
SOD	SOF	SOS	SSF	SSY	STF	STI
STO	STT	STW	SVV	SZR	TER	THO
TOL	TON	TSC	TUN	UEI	UFI	UOS
UOV	UOZ	USI	UTL	UWY	VET	VFI
VNI	VSV	WEI	YUG	ZON		

SI1.2 Top Candidates from Deem's Database

2-dimensional channel system:
8056830
8080784
8087188
8206103
8206155
8206186
8214411
8255418
8265201
8265611
8265828
8267423
8268490
8268700
8274307
8283850
8287620
8287803
8289148
8289716
8292668
8292962
8293280
8312155
8312223
8313037
8313042
8315144
8318459
8319320
8321874
8322959
8325096
8326559
8326730
8326866
8329937
3-dimensional channel system:
8067418
8078629
8084708
8133379

8194023
8268600
8286937
8287056
8298667
8301472
8307693
8312978
8315436
8315703
8316304
8316376
8317141
8317769
8318323
8318347
8323183
8323211
8323836
8324002
8325000
8326122
8326877
8328497
8328498
8328529
8329212
8329795
8331121

SI1.3 Alternative Filter Funnel

In an initial screening, we used a filter funnel that was slightly different. First, the LIDs criteria were trained including RWY. Second, the tetrahedrality criteria were trained on five instead of 7 industrially important frameworks:[S1] BEA, CHA, FAU, MFI, and MOR. The results of this funnel are given in Figure S1 and the below list of top candidates, which is much shorter than our list given above.

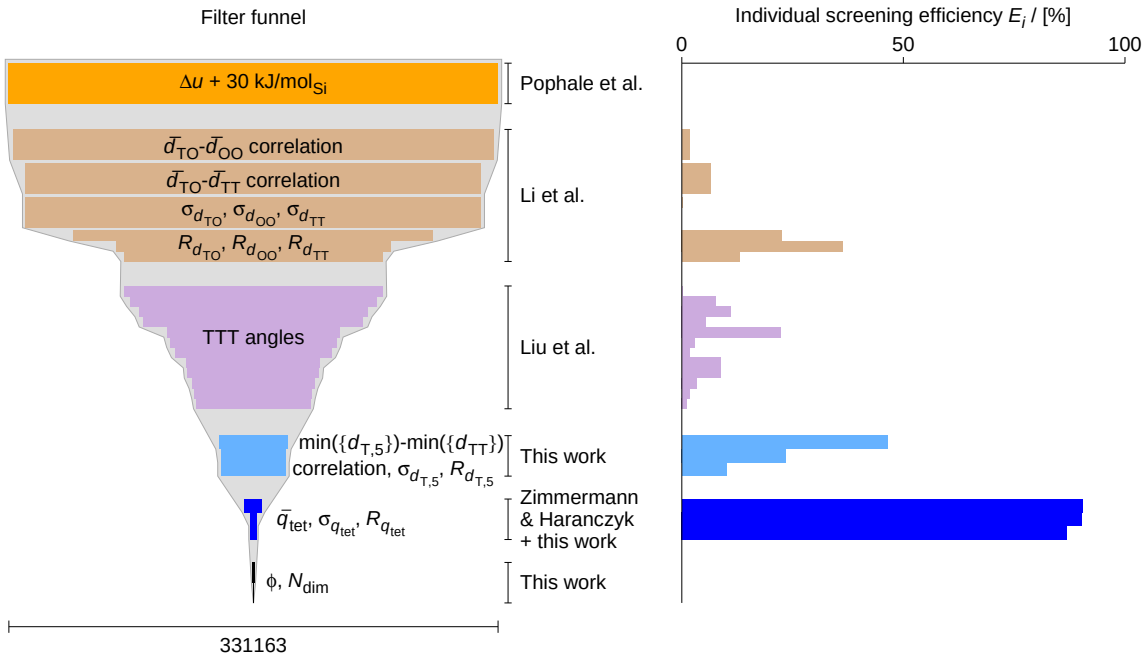

Figure S1: Left: alternative filter funnel; number of remaining hypothetical zeolite structures after each screening step, resulting in a total screening efficiency of at least $E = 100 \times (331163 - 30)/331163 = 99.9909\,\%$. Right: screening efficiencies of each individual filter step separately, E_i.

Top candidates from Deem's database using the alternative filter funnel: 2-dimensional channel system:
8116500
8292668
8315144
8326559
8321874
8265611
8206103
8329937
8214411
8289148
8313037

8268490
8325096
3-dimensional channel system:
8317769
8194023
8286937
8312978
8078629
8328529
8323211
8268600
8323183
8133379
8325000

SI2 List of symbols

Symbol	Description	Units
$C_{i,j}$	j-th fit parameter of criterion/correlation i	–
d	(interatomic) distance	Å
E	(overall) screening efficiency (of a collection of filters)	–
E_i	screening efficiency of filter i	–
i	index variable	–
j	index variable	–
$\mathcal{L}$	likelihood	–
N	number of structures	–
N	Absolute frequency	–
N_{descr}	number of descriptors	–
N_{dim}	channel dimensionality	–
N_i	number of structures left after filter step i	–
N_{input}	number of structures which enter a filter (or a collection of filters)	–
N_{T}	number of T-atoms in a given ring	–
p	relative frequency	–
q_{tet}	tetrahedral order parameter (here also called tetrahedrality)	–
R	range of a set of values X (i.e., $\max(\{X\}) - \min(\{X\})$)	–
u	lattice energy of a material	kJ (mol Si)$^{-1}$
u	lattice energy	kJ (mol Si)$^{-1}$
Δu	lattice energy relative to α-quartz	kJ (mol Si)$^{-1}$
δu	threshold lattice energy	kJ (mol Si)$^{-1}$
$\bar{x}$	average x-value in a structure	–

To be continued on next page.

Symbol	Description	Units
α	T-atom ring angle	$^\circ$
α^i	(average) angle in a ring with i T-atoms	$^\circ$
ε_i	absolute (y-axis) deviation from a regression line	–
ϕ	porosity	–
μ_i	expectation value of property i	–
ϑ	feasibility factor	–
ρ_{FW}	framework density	T-atoms (1000 Å^3)$^{-1}$
σ_i	standard deviation of quantity i	–

Subscript	Description
industry	relates to the 5 industrially most important zeolites (BEA, CHA, FAU, MFI, MOR)
IZA	relates to the IZA database
TO	relates to T–O bonds
TT	relates to T neighbors of a central T-atom that are 2 consecutive T–O bonds away (i.e., T–O–T)
T,5	relates to 5th-nearest neighbor of a given T-atom
OO	relates to O neighbors of a central O-atom that are 2 consecutive T–O bonds away (i.e., O–T–O)

Acronym or Abbreviation	Description
ADOR	assembly disassembly organization reassembly
DLS	distance least squares
IZA	International Zeolite Association
GULP	General Utility Lattice Program
LID	local interatomic distance
MC	Monte Carlo
SLC	Sanders–Leslie–Catlow (force field)

References

(S1) Zimmermann, N. E. R.; Haranczyk, M. History and utility of zeolite framework-type discovery from a data-science perspective. *Cryst. Growth Des.* **2016**, *16*, 3043–3048.