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Supporting Information: Predicting low-k zeolite materials

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I. DFT CALCULATIONS

We use the VASP (Vienna Ab initio Simulation Package) code[1] and PBE functional[2] with a planewave basis set and the all-electron-like projector augmented wave (PAW) method[3] for core electrons and ionic potentials. The static dielectric constant is computed using perturbation theory (density functional perturbation theory (DFPT)) and the methodology proposed in Ref. 4. Local fields effects are computed including both changes in the Hartree potential and the exchange and correlation potential. The ionic contribution to the dielectric constant is computed using the methodology proposed in Ref. 5. We use a planewave energy cutoff of 600 eV for all zeolites and a Monkhorst-Pack mesh up to $5\times5\times5$ for the Brillouin zone integration (for larger unit cell we use a spaser grid). In order to compute the relaxed-ion static dielectric tensor and the elastic constants, we performed a structural relaxation of all computed zeolites. Starting from the structures found in the IZA database, the atomic positions and the lattice vectors are relaxed until the residual forces are smaller than 0.01 eV/Å and the stress tensor components are smaller than 0.2 kbar. The elastic tensor is computed by performing six finite distortions ($\pm$ 0.015 Å) of the lattice followed by a full atomic relaxation. The elastic constants are derived using the stress-strain relationship based on the generalized Hooke's law.

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Zeolite	classical (GULP) k	DFPT k
LTA	2.72	2.95
EDI	3.10	3.41
LOV	3.16	3.57
ATT	3.30	3.42
ASV	3.53	3.86
ABW	3.52	3.81
GON	3.54	4.03
CAS	3.92	4.2
BCT	3.98	4.10

TABLE I. Dielectric constant (sum of electronic and ionic contributions) computed using GULP and VASP for a few IZA structures. We have selected structures with sufficiently different k values obtained with GULP and relatively small unit cell ($<$ 100 atoms) to run the DFPT calculations.

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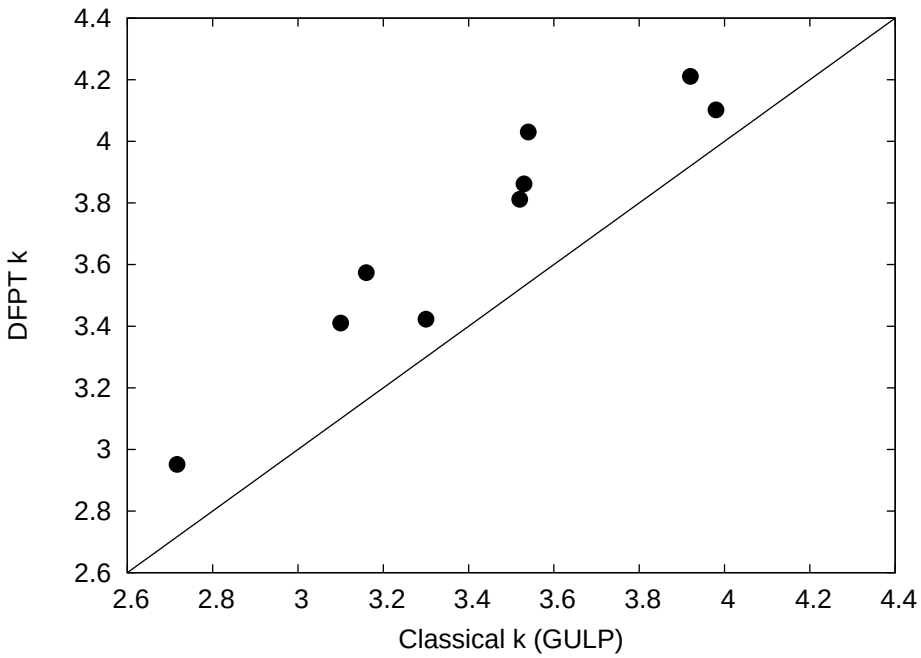

Figure S 1. DFPT k plotted over the GULP k values for a few IZA zeolites. A good correlation between DFPT and GULP k is found.

Zeolite	B (GPa) classical (GULP)	B(GPa) DFT
RWY	3.2	13.1
VET	52.8	31.3
SOS	56.3	47.5
FER	100.5	93.3
BCT	135.5	128.4

TABLE II. Bulk modulus computed using GULP and VASP for a few zeolites. As for the dielectric constant, we have selected structures with different values of B obtained with GULP. A reasonable agreement is found between the classical model and DFT.

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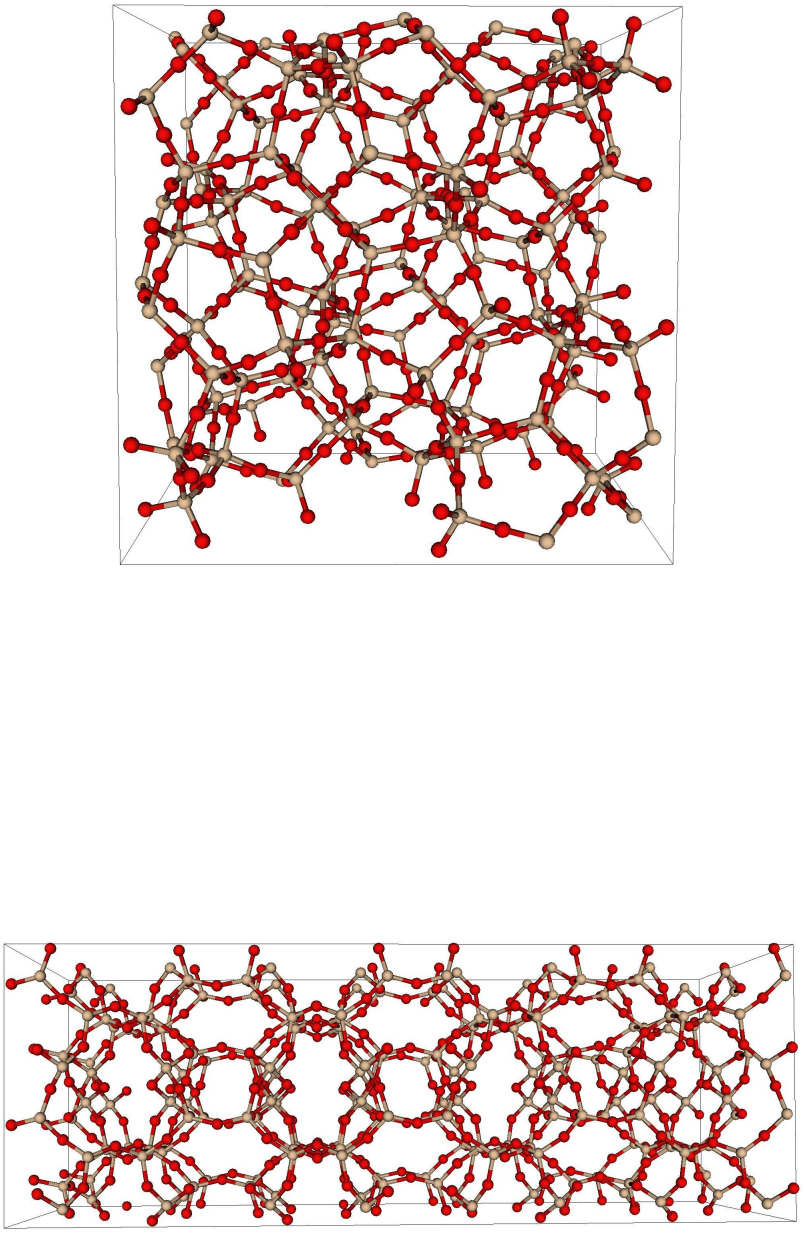

Figure S 2. Unit cell representation of MTN (upper panel) and SOS (lower panel) zeolites. MTN has a homogoneous distribution of the silicon and the oxygen atoms while SOS exhibits large pores separated by homogeneous networks. Our analysis shows that the zeolites similar to MTN tend to have higher k compared to zeolites similar to SOS.

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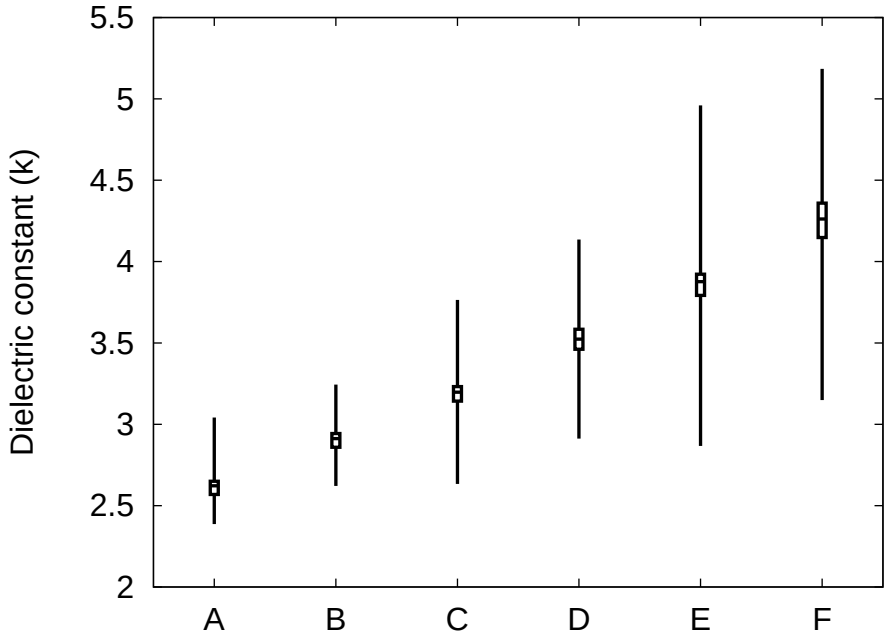

Figure S 3. Box plot of k computed for 1200 zeolite structures in the hypothetical zeolite database. Groups A, B, C, D, E, and F, correspond to framework densities of 1285-1315 kg/m^3, 1485-1515 kg/m^3, 1685-1715 kg/m^3, 1885-1915 kg/m^3, 2085-2115 kg/m^3, and 2285-2315 kg/m^3, respectively. A significant increase in spread from group A (k = 2.62$\pm$0.09) to group F (k = 4.26$\pm$0.21) is found.

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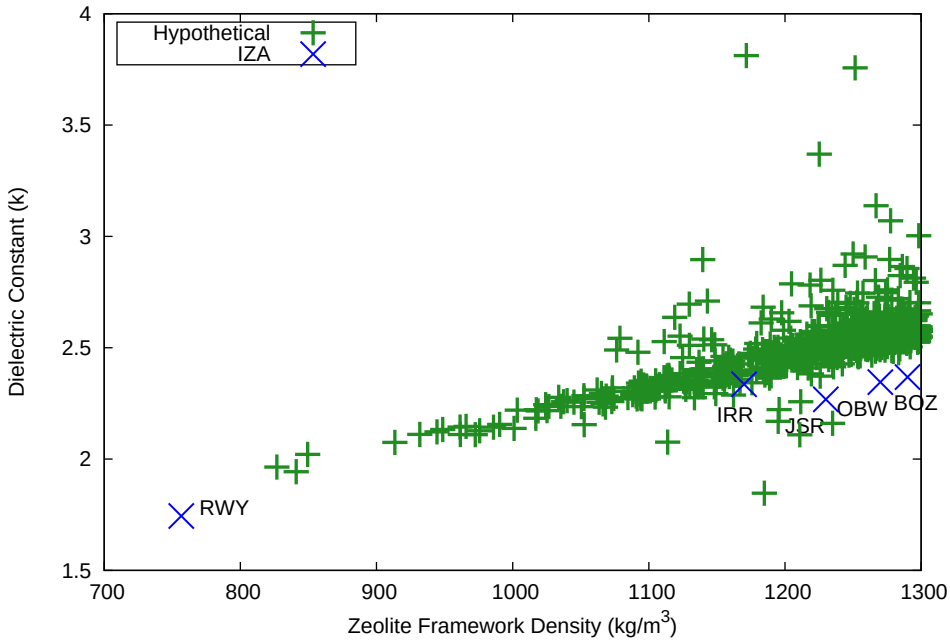

Figure S 4. Dielectric constant k as a function of FD for zeolites with FD < 1300 kg/m^3. 770 structures in the hypothetical zeolite database and five IZA structures (RWY, IRR, JSR, OBW, and BOZ) are included. A positive correlation betwen k and FD is shown, similar to the IZA case (Figure 1 of the manuscript).

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Zeolite	static k	high freq. k	B (GPa)
RWY	1.74	1.29	3.2
JSR	2.27	1.44	47.0
OBW	2.34	1.47	65.1
IRR	2.33	1.42	42.1
BOZ	2.37	1.47	57.6
OSO	2.39	1.48	64.6
NPT	2.49	1.50	72.9
JST	2.53	1.52	4.1
ITT	2.57	1.47	51.0
TSC	2.64	1.50	63.9
FAU	2.65	1.50	62.7
EMT	2.65	1.50	62.4
SBT	2.66	1.51	58.8
SBS	2.66	1.51	59.0
SAO	2.68	1.53	62.7
SBE	2.70	1.51	65.9
LTA	2.72	1.54	76.1
MEI	2.73	1.55	63.3
PUN	2.78	1.56	54.6
IWS	2.81	1.55	62.1
AFY	2.81	1.52	53.7
AFS	2.82	1.55	68.8
BPH	2.82	1.55	68.8
BEC	2.85	1.57	66.4
ISV	2.85	1.57	69.6
DFO	2.86	1.56	64.3
SFO	2.87	1.57	62.5
AFR	2.87	1.57	63.7

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Zeolite	static k	high freq. k	B (GPa)
UFI	2.88	1.58	72.5
WEI	2.88	1.62	60.9
SOS	2.91	1.62	56.3
RHO	2.91	1.56	75.6
BEA	2.92	1.58	69.1
ETR	2.92	1.58	45.3
NAB	2.93	1.61	89.6
JOZ	2.95	1.62	63.5
AFX	2.95	1.58	79.6
AEI	2.95	1.58	80.1
AFT	2.95	1.58	79.5
CHA	2.95	1.58	80.1
IWR	2.96	1.60	68.7
SAV	2.99	1.57	79.1
SBN	3.00	1.62	93.8
RTH	3.00	1.62	69.1
STW	3.00	1.62	67.0
UTL	3.02	1.59	55.4
IWV	3.03	1.57	71.7
ITE	3.03	1.61	73.7
USI	3.03	1.60	56.2
CON	3.04	1.60	68.7
SAS	3.06	1.59	80.3
EDI	3.07	1.63	97.8
BOG	3.08	1.61	68.9
ERI	3.08	1.62	87.5
OFF	3.08	1.62	87.1
NAT	3.08	1.63	97.8

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Zeolite	static k	high freq. k	B (GPa)
MWW	3.09	1.61	78.9
VFI	3.10	1.55	79.1
MSE	3.10	1.63	74.6
CGS	3.11	1.64	39.0
LTL	3.11	1.63	62.4
UWY	3.11	1.63	73.3
LEV	3.12	1.62	86.4
AST	3.12	1.62	102.9
EAB	3.13	1.62	85.3
PAU	3.13	1.62	82.8
STT	3.15	1.65	45.5
THO	3.15	1.62	93.0
STI	3.15	1.64	80.9
ACO	3.15	1.65	104.4
SAT	3.15	1.64	87.6
MOZ	3.16	1.65	68.0
LOV	3.16	1.65	95.9
IFR	3.16	1.66	52.0
AWW	3.16	1.66	72.7
ATS	3.16	1.63	84.1
SEW	3.17	1.65	55.2
PHI	3.17	1.64	79.8
SIV	3.17	1.64	78.2
MER	3.18	1.64	80.0
EZT	3.18	1.66	55.8
IWW	3.19	1.63	54.9
RSN	3.19	1.65	96.4
ZON	3.19	1.69	47.6

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Zeolite	static k	high freq. k	B (GPa)
SFS	3.20	1.64	68.0
JSN	3.20	1.69	54.2
GIS	3.20	1.64	87.3
SSF	3.21	1.64	82.4
OKO	3.22	1.68	54.8
VSV	3.23	1.65	96.8
UOS	3.23	1.68	81.1
DON	3.24	1.66	43.0
RTE	3.24	1.67	75.9
LTN	3.24	1.66	72.6
NPO	3.25	1.72	22.0
LTF	3.26	1.64	84.6
TOL	3.26	1.70	40.2
HEU	3.27	1.68	67.0
SVV	3.27	1.70	36.2
ITH	3.27	1.67	66.6
ITR	3.27	1.67	68.8
AFN	3.27	1.67	65.3
STF	3.27	1.65	71.4
SFF	3.28	1.68	31.9
SFN	3.29	1.64	80.0
LIO	3.29	1.69	62.3
VNI	3.29	1.68	65.7
OWE	3.29	1.67	91.9
ESV	3.29	1.69	23.6
SGT	3.29	1.69	67.9
MAZ	3.30	1.65	88.7
SFH	3.30	1.64	83.1

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Zeolite	static k	high freq. k	B (GPa)
ATT	3.30	1.67	93.0
GIU	3.31	1.68	102.9
DDR	3.31	1.70	46.0
IFO	3.32	1.66	44.3
MAR	3.32	1.69	60.1
FAR	3.32	1.68	104.4
CAN	3.32	1.67	108.7
AFG	3.33	1.67	109.6
ITW	3.33	1.69	88.6
LOS	3.34	1.67	109.9
SOF	3.35	1.63	67.1
RUT	3.35	1.71	44.0
SFV	3.35	1.68	57.8
EON	3.36	1.66	88.6
TER	3.37	1.67	86.9
TUN	3.38	1.68	51.7
PON	3.38	1.70	61.8
MFI	3.38	1.71	40.0
NES	3.38	1.64	88.7
MEL	3.38	1.68	81.4
LAU	3.39	1.70	65.4
BRE	3.39	1.71	62.5
SFG	3.39	1.69	74.1
SOD	3.39	1.67	111.0
CFI	3.40	1.66	97.4
CDO	3.40	1.72	97.7
IMF	3.41	1.68	72.7
AFI	3.41	1.67	97.7

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Zeolite	static k	high freq. k	B (GPa)
RRO	3.42	1.69	69.8
MSO	3.42	1.70	81.4
BOF	3.43	1.71	64.7
APC	3.43	1.70	92.4
UOZ	3.43	1.75	43.6
STO	3.44	1.73	46.6
CGF	3.44	1.73	23.3
ATN	3.44	1.71	92.8
MOR	3.45	1.67	92.9
JSW	3.46	1.72	84.3
SZR	3.46	1.69	94.5
EUO	3.46	1.68	83.4
AWO	3.47	1.71	86.1
OSI	3.47	1.70	103.5
GOO	3.47	1.73	44.1
DFT	3.47	1.70	109.6
AET	3.48	1.70	39.3
MTW	3.50	1.72	70.9
UEI	3.50	1.69	91.6
SFE	3.51	1.67	90.3
SSY	3.51	1.67	91.7
YUG	3.51	1.71	90.9
IHW	3.51	1.72	57.3
ABW	3.52	1.70	114.1
SAF	3.52	1.74	59.6
LTJ	3.53	1.73	93.3
MFS	3.53	1.69	90.9
ASV	3.53	1.74	60.7

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Zeolite	static k	high freq. k	B (GPa)
BSV	3.53	1.70	81.1
DAC	3.54	1.69	99.6
GON	3.55	1.74	38.6
DOH	3.56	1.69	119.4
AFO	3.56	1.76	64.2
EPI	3.58	1.70	96.6
FER	3.58	1.70	100.5
JRY	3.58	1.73	93.3
APD	3.61	1.72	114.1
MEP	3.65	1.73	103.3
MON	3.65	1.70	107.3
RWR	3.66	1.77	103.8
MTN	3.66	1.70	125.4
AEL	3.66	1.76	54.5
ATO	3.67	1.74	94.7
MRE	3.67	1.78	57.2
FRA	3.68	1.65	101.0
NON	3.68	1.71	116.7
ANA	3.70	1.77	106.9
VET	3.71	1.79	52.8
PCR	3.72	1.74	65.9
TON	3.75	1.73	103.8
MTT	3.75	1.73	100.8
JBW	3.75	1.76	112.6
AHT	3.77	1.75	104.4
SFW	3.78	1.54	34.4
AEN	3.87	1.80	95.0
MTF	3.87	1.82	51.0

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Zeolite	static k	high freq. k	B (GPa)
ATV	3.88	1.77	124.3
CAS	3.92	1.76	121.7
NSI	3.93	1.76	123.7
CZP	3.93	1.82	51.6
BIK	3.95	1.76	123.1
BCT	3.97	1.78	135.3
MVY	4.67	1.82	84.9

TABLE III. Static dielectric constant, high frequency dielectric constant, and bulk modulus for the 205 IZA zeolite structures.