

# **SUPPLEMENTARY INFORMATION**

**for**

## **A Systematic Typology for Negative Poisson's Ratio Materials and the Prediction of Complete Auxeticity in Pure Silica Zeolite JST**

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## I. Auxeticity in cubic systems

The necessary and sufficient conditions for complete auxeticity in a cubic crystal are

$$C_{12} < 0 \text{ and } \frac{C_{44}}{C_{11}} \geq \frac{C_{44}}{C_{11}} \left( \frac{1}{2} - \frac{C_{12}}{C_{11}} \right) + \frac{1}{2} \quad [1].$$

These conditions are depicted in Figure S1.

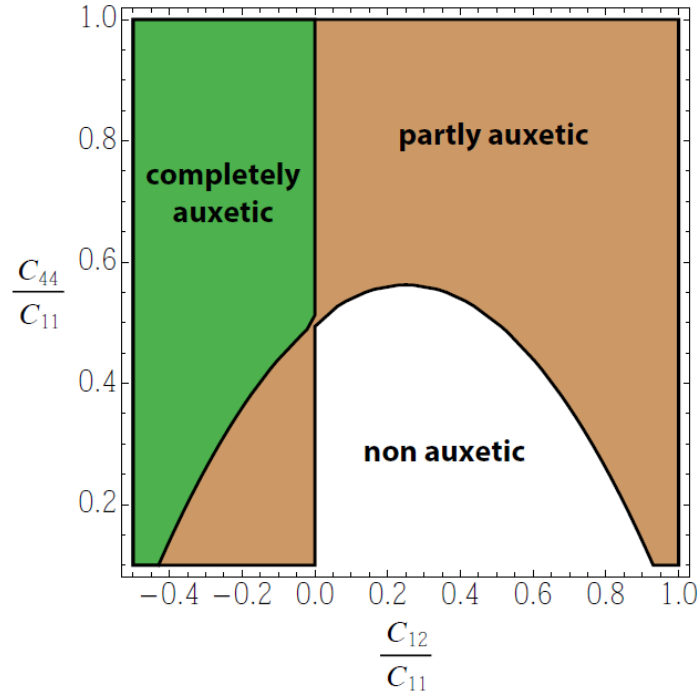


Figure S1. Auxeticity map for cubic systems

## II. Potential Validation

Table S1(a) – Comparison of lattice parameters and elastic constants with experimental data; quartz

	Exp.	Catlow	Gale	Sastre	BKS	Matsui	DFT
a (Å)	4.91	4.84	4.97	4.90	4.92	5.02	5.12
c (Å)	5.41	5.34	5.49	5.43	5.45	5.56	5.62
RMSE (Å)	0	0.07	0.07	0.02	0.03	0.13	0.21
$C_{11}$ (GPa)	87.64	94.6	91.1	83.5	88.9	71.1	112.7
$C_{12}$ (GPa)	6.99	18.4	9.0	20.2	9.2	9.7	34.8
$C_{13}$ (GPa)	11.91	19.7	14.5	30.3	15.7	12.4	40.3
$C_{14}$ (GPa)	-17.19	-14.5	-16.7	-10.1	-17.1	-13.9	4.9
$C_{33}$ (GPa)	107.2	116.1	103.3	100.5	110.4	93.0	163.5
$C_{44}$ (GPa)	57.94	50.0	46.7	40.4	50.9	40.4	65.2
$C_{66}$ (GPa)	39.88	38.1	41.0	31.6	39.8	30.7	38.9
RMSE (GPa)	0	7.6	5.0	11.9	3.5	11.1	29.2

Table S1(b) – Comparison of lattice parameters and elastic constants with experimental data; cristobalite

	Exp.	Catlow	Gale	Sastre	BKS	Matsui	DFT
a (Å)	4.96	4.97	5.14	5.00	4.91	5.18	5.27
c (Å)	6.91	7.01	7.22	7.14	6.56	7.04	7.45

RMSE (Å)	0	0.07	0.25	0.17	0.24	0.19	0.44
C <sub>11</sub> (GPa)	59.45	74.3	73.2	61.8	68.2	52.7	95.5
C <sub>12</sub> (GPa)	3.88	4.4	3.2	1.6	10.6	8.7	7.4
C <sub>13</sub> (GPa)	-4.49	9.6	6.8	17.7	1.8	0.6	4.0
C <sub>33</sub> (GPa)	42.47	69.2	63.4	60.8	44.9	38.1	53.2
C <sub>44</sub> (GPa)	67.24	74.7	74.11	64.0	71.7	58.4	71.4
C <sub>66</sub> (GPa)	25.74	30.0	29.82	18.7	25.0	18.4	22.9
RMSE (GPa)	0	14.2	11.7	12.2	5.6	6.4	15.9

Table S1(c) – Comparison of lattice parameters and elastic constants with experimental data; MFI

	Exp.	Catlow	Gale	Sastre	BKS	Matsui
a (Å)	20.09	20.07	20.46	20.18	20.34	20.91
b (Å)	19.74	19.69	20.24	19.85	20.32	20.86
c (Å)	13.14	13.35	13.65	13.45	13.67	14.03
RMSE (Å)	0	0.12	0.46	0.20	0.47	0.95
C <sub>11</sub> (GPa)	84.5	104.9	136.8	99.1	37.6	31.6
C <sub>12</sub> (GPa)	-1.52	12.0	33.1	16.8	14.4	11.5
C <sub>13</sub> (GPa)	19.9	32.1	56.6	36.8	-1.2	-0.3
C <sub>22</sub> (GPa)	68.2	68.3	99.6	59.4	81.8	71.0
C <sub>23</sub> (GPa)	10.3	17.6	37.0	23.1	25.1	21.0
C <sub>33</sub> (GPa)	79	76.0	107.3	73.7	81.2	68.0
C <sub>44</sub> (GPa)	22.6	33.8	16.5	31.4	19.3	16.6
C <sub>55</sub> (GPa)	23.5	29.7	26.3	15.9	20.2	16.5
C <sub>66</sub> (GPa)	21.2	23.0	21.9	16.2	20.6	17.0
RMSE (GPa)	0	10.4	29.5	11.9	19.2	20.3

### III. Bibliography

- [1] A. Brańka, D. Heyes, and K. Wojciechowski, Phys. Status Solidi B **246**, 2063 (2009).