Supporting Information for:

Isomorphism of anhydrous tetrahedral halides and silicon chalcogenides; energy landscape of crystalline BeF_2, $BeCl_2$, SiO_2 and SiS_2.

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S1. Comparison of the PBE0 calculated and experimentally measured[1] frequencies of the longitudinal phonons in siliceous quartz.

A1	
Calc	Exp
226	207
338	356
462	464
1097	1085

$A2_T$	
Calc	Exp
344	364
492	495
787	778
1089	1080

E_T	
Calc	Exp
134	128
257	265
386	394
441	450
703	697
809	795
1080	1072
1167	1162

S2. PBE0 optimised crystal structure for BeF_2 Coesite.

BeF_2 Coesite
Space group C2/C (15)
Cell parameters
6.97192 12.02685 6.96194 90.000 120.020 90.000
Fractional atomic coordinates
Be 0.141484 0.107488 0.072694
Be -0.494856 0.158541 -0.461605
F 0.000000 0.256085 0.000000
F 0.500000 0.121460 -0.250000
F 0.274976 0.120461 -0.051015
F 0.307365 0.107014 0.327423
F 0.011053 0.212034 0.482707

[1] Scott, J.F.; Porto, S.P.S. Phys. Rev. **1967**, 161, 903.

S3. PBE0 optimised crystal structure for low energy porous BeF_2 materials.

BeF_2 SOD
Space group P-43n (218)
Cell parameters
8.529749 8.529749 8.529749 90.000 90.000 90.000
Fractional atomic coordinates
Be 0.250000 -0.500000 0.000000
Be 0.250000 0.000000 -0.500000
F 0.145401 0.145401 -0.467069

BeF_2 CHA
Space group R-3m (166)
Cell parameters
13.128497 13.128497 14.429386 90.000 90.000 120.000
Fractional atomic coordinates
Be 0.229790 -0.000114 0.103189
F 0.119514 -0.119514 0.127063
F 0.333333 0.019843 0.166667
F 0.200699 0.100340 0.118040
F 0.264807 0.000000 0.000000

S4. PBE0 optimised crystal structure for low energy porous $BeCl_2$ materials.

$BeCl_2$ RWY
Space group I-43m (217)
Cell parameters
19.781456 19.781456 19.781456 90.000 90.000 90.000
Fractional atomic coordinates
Be 0.067715 0.191483 -0.452279
Cl 0.134510 0.134510 -0.398399
Cl -0.382048 -0.249818 -0.019895
Cl -0.500000 -0.369319 -0.000000

$BeCl_2$ OSO
Space group $P3_2$ (145)
Cell parameters
11.515934 11.515934 8.400845 90.000 90.000 120.000
Fractional atomic coordinates
Be -0.442609 0.294831 -0.250204
Be 0.294778 -0.442646 0.032580
Be 0.000024 0.411549 0.224572
Cl -0.276468 0.299843 -0.345897
Cl 0.276523 -0.423755 -0.205101
Cl 0.381683 0.142613 -0.339741
Cl 0.457605 -0.462732 0.076558

Cl 0.142535 0.381625 0.121974
Cl -0.462957 0.457528 -0.294041

$BeCl_2$ SOD
Space group P-43n (218)
Cell parameters
9.845269 9.845269 9.845269 90.000 90.000 90.000
Fractional atomic coordinates
Be 0.250000 0.500000 0.000000
Be 0.250000 0.000000 0.500000
Cl 0.134415 0.134415 -3.927462