Supplementary Information for

Ab Initio Investigation of the Respective Stability of Silicogermanates and Their (Alumino)Silicates Counterparts

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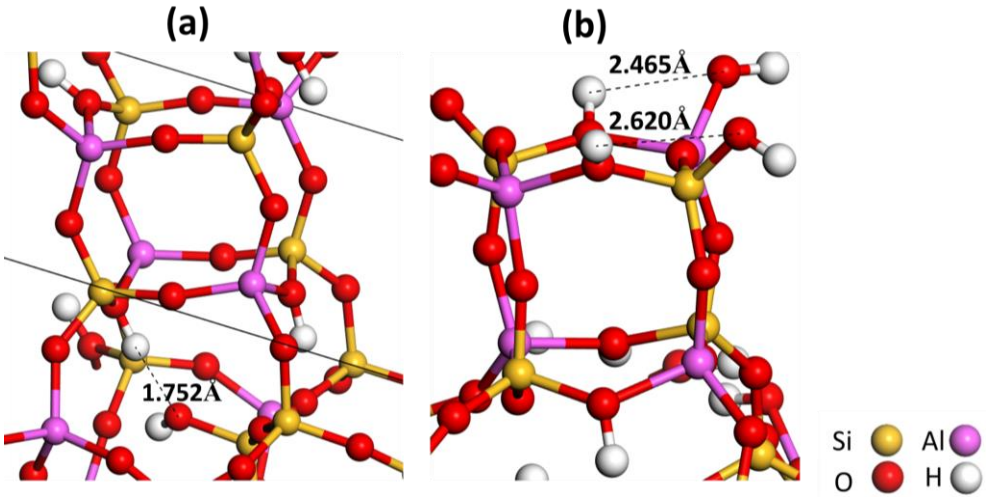

Figure S 1: Interactions between hydroxyls of interrupted frameworks and compensation hydrogen atoms illustrated with dashed lines inside an –IRY (a) and location of the interrupted sites on the d4r units of the –ITV (b) aluminosilicate structures.

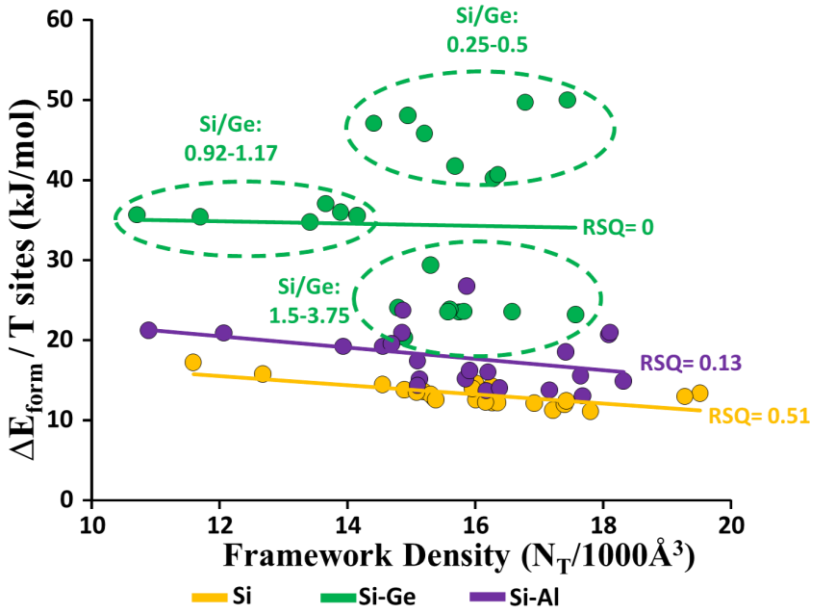

Figure S 2: Framework density effect on the energies of formation per T sites (ΔE_{form}/T sites) of normal and disordered silicates (yellow), silicogermanates (green) and aluminosilicates (purple). Si, Si-Ge and Si-Al represent silicates, silicogermanates with Ge occupying the full d4r and aluminosilicates respectively. Si/Ge is the ratio of T sites occupied by Si over the T sites occupied by Ge.

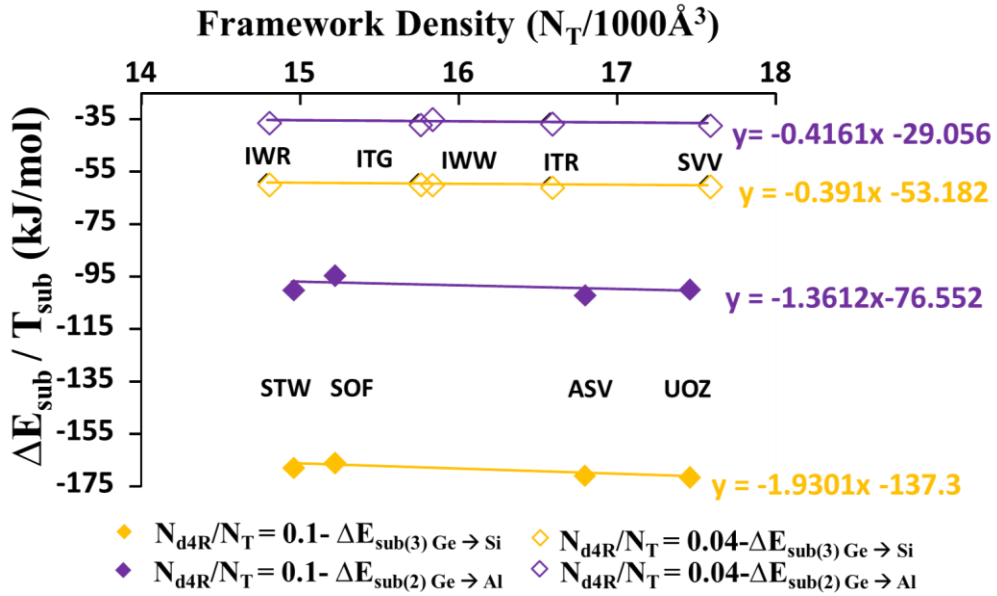

Figure S 3: Energies of full substitution of Ge for Si $\Delta E_{sub\ (3),\ Ge \rightarrow Si}$ (yellow) and of Ge for Al $\Delta E_{sub\ (2),\ Ge \rightarrow Al}$ (purple) normalized to the number of substituted T sites against the framework density of regular and disordered structures having a number of d4r over the number of T sites (N_{d4r}/N_T) equal to 0.04 and 0.1.

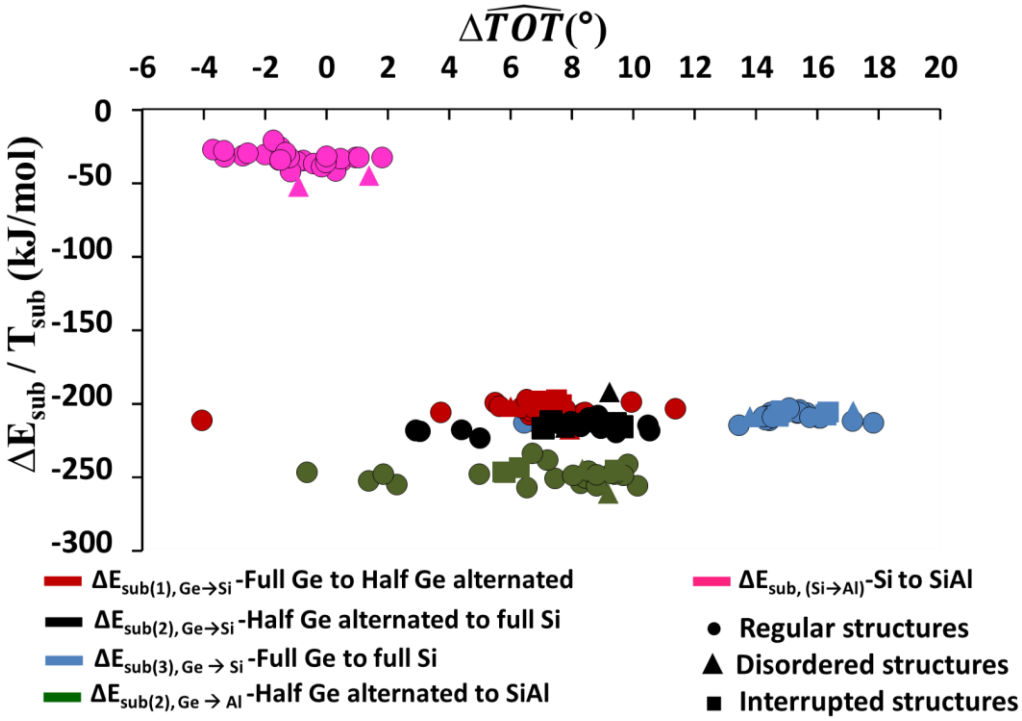

Figure S 4: Energies of substitution per T substituted atoms (ΔE_{sub} / T_{sub}) of : Ge for Si departing from Ge occupying the full d4r to half Ge alternated, departing from half Ge alternated to full silicate and from full Ge in the d4r to full silicate respectively. Substitution of Ge for Al $\Delta E_{sub\ (2),\ Ge \rightarrow Al}$ departing from Ge occupying half of the d4r with alternation. $\Delta E_{sub\ ,\ Si \rightarrow Al}$ departing from full silicate to aluminosilicate with Al alternated in the d4r . $\Delta\widehat{TOT}$corresponds to the difference of angles in the d4r between the initial and the substituted zeolite.

Table S 1: Cell parameters (Å) of the silicates, silicogermanates and aluminosilicates after geometry optimization compared to those of silicates from IZA. Full d4r is for Ge occupying all the d4r. Half d4r alternated and same s4r stand for Ge occupying half of the d4r.

	IZA			Our Work														
	Silicates			Silicates			Silicogermanates									Aluminosilicates		
							Full d4r			half d4r alternated			half d4r same s4r					
IZA Structural code	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c	a	b	c
Regular	**(Å)**																	
ASV [1]	8.6740	8.6740	13.9190	8.5391	8.5391	14.0510	8.9752	8.9752	14.7923	8.7840	8.7840	14.3924	8.7652	8.7652	14.4190	8.7496	8.7575	14.4425
BEC [2-5]	12.7690	12.7690	12.9770	12.7266	12.7266	13.2642	13.1611	13.1611	13.5239	12.9157	12.9157	13.4315	12.8997	12.8997	13.4288	12.9507	12.9194	13.1423
IRN [6]	19.6410	18.4574	16.5655	19.6901	18.5225	16.5971	19.8466	19.0400	16.8880	19.7294	18.8323	16.8557	19.8522	18.4307	16.6603	20.0586	18.4247	16.7568
IRR [7-10]	19.0315	19.0315	14.1008	19.1114	19.1114	14.1854	19.6899	19.6899	14.4623	19.3771	19.3771	14.3434	19.2890	19.2890	14.3832	19.6551	19.6723	14.2587
ITG [11]	12.7411	12.6989	20.9990	12.9355	12.6285	21.2287	13.0406	12.8463	21.3936	13.0568	12.7432	21.3630	13.0685	12.7059	21.3060	12.9175	12.6904	21.2452
ITR [12,13]	11.6731	21.9694	25.1700	11.6967	22.0197	25.2513	11.7094	22.2538	25.9255	11.6960	22.2778	25.6261	11.6490	22.2854	25.5777	11.6741	22.0816	25.3156
ITT [14-20]	18.8677	18.8677	11.6332	19.0036	19.0036	11.5999	19.6196	19.6196	11.7960	19.2797	19.2797	11.6989	19.1851	19.1851	11.7224	19.4339	19.5478	11.5352
IWR [21-23]	21.2325	13.3024	12.6759	21.3018	13.5395	12.6384	21.5229	13.6520	12.8832	21.4207	13.6187	12.7514	21.3753	13.6232	12.7520	21.3755	13.6705	12.6650
IWS [24]	26.6887	26.6887	12.9078	26.7203	26.7203	13.0905	27.5967	27.5967	13.3114	27.1877	27.1877	13.1929	27.1398	27.1398	13.2054	27.5693	27.1794	13.0225
IWW [25-28]	41.6908	12.7128	12.7114	41.9895	12.9274	12.6176	42.3461	12.9871	12.8716	42.2909	13.0128	12.7576	42.2601	12.9995	12.7531	41.9854	13.0009	12.6640
POS [29]	18.7661	18.7661	11.6939	18.8915	18.8915	11.7177	19.4848	19.4848	11.9075	19.2808	19.2808	11.7886	19.1773	19.1773	11.8230	19.4205	19.3366	11.5988
SOF [30]	20.3320	12.0850	10.2750	20.3769	12.1399	10.3166	21.0154	12.4216	10.4959	20.7459	12.4079	10.4055	20.5677	12.4386	10.3310	20.5641	12.7309	10.1052
SOR [31,32]	20.9277	17.7028	7.5877	21.0668	17.6975	7.6058	21.5708	17.9270	7.9124	21.1697	17.5305	7.6290	21.1695	17.8490	7.7304	21.3027	16.4875	7.7436
SOV [33]	24.6308	26.6513	12.7267	24.9330	26.7684	12.7135	25.4342	27.6301	13.1088	24.9937	27.1820	12.8815	24.8066	26.9108	12.8471	24.6183	26.9371	12.7876
STW [30,34]	11.8870	11.8870	29.9150	11.9763	11.9763	30.1764	12.4297	12.4297	29.9990	12.3254	12.2758	30.0190	12.2454	12.2454	30.2563	12.3195	12.4651	30.4254
SVV [35,36]	13.1231	13.3734	21.2620	13.1705	13.4646	21.2644	13.1966	13.5708	21.3174	13.1884	13.5233	21.3138	13.1746	13.5061	21.2746	13.2418	13.4432	21.3533
UOS [37]	19.9055	7.5460	9.0683	19.9300	7.5968	9.1090	20.2589	7.8924	9.2181	20.0633	7.7684	9.1687	20.0053	7.7975	9.1947	19.3528	7.8895	9.0259
UOV [38]	12.7177	21.9894	38.7639	12.6650	22.2428	39.0242	12.7792	22.4314	39.3458	12.7303	22.3919	39.2935	12.7444	22.3780	39.2229	12.7466	22.2840	39.0861
UOZ [39]	8.6209	8.6209	27.5436	8.5935	8.5935	28.0896	8.7429	8.7429	29.9963	8.7273	8.7273	28.5131	8.7135	8.7135	28.5133	8.8007	8.7976	28.5289
UTL [40-43]	28.9964	13.9679	12.4493	29.2404	14.0346	12.4635	29.9209	14.0598	12.5173	29.5463	14.0410	12.4941	29.6826	14.0503	12.4792	29.7284	14.0340	12.4699
UWY [44]	25.1100	12.7330	11.5100	25.1748	12.7273	11.5827	25.5940	12.9532	11.8285	25.4689	12.8422	11.7282	25.3311	12.7911	11.6336	25.3295	12.9291	11.5167
Interrupted																		
-IFT [45]	18.8890	22.8023	29.0815	19.0045	22.9209	29.2772	19.5648	23.0719	29.2611	19.4203	22.9662	29.2354	19.3083	22.9395	29.2218	19.4249	22.9129	29.2951
-IFU [46]	26.0358	25.5895	15.8248	26.1672	25.5710	15.9071	27.2750	26.0285	16.5553	26.8986	25.6463	16.2519	26.9349	25.5510	16.2793	27.2073	25.7455	16.5565
-IRY [47]	15.9499	15.9499	31.0796	16.0892	16.0512	31.1723	16.7768	16.6956	31.6519	16.4751	16.4020	31.4939	16.4121	16.3428	31.4940	16.6219	16.5544	31.4156
-ITV [8,48-50]	26.3099	26.3099	26.3099	26.3047	26.3073	26.3073	26.2979	26.3342	26.3342	26.3002	26.3352	26.3547	26.2999	26.3294	26.3200	26.4294	26.1581	26.4098
Partially Disordered																		
***CTH [51-54]**	10.4578	27.7607	27.2023	10.4433	27.9143	27.5152	10.4065	27.9272	28.2821	10.1470	27.7089	27.7765	10.1088	27.6222	27.7870	10.1022	27.6753	27.9439
***UOE [55]**	9.0869	7.5548	10.4761	9.0996	7.5859	10.5026	9.2092	7.8734	10.5289	9.1499	7.7130	10.5323	9.0589	7.7526	10.3265	8.7640	8.7640	10.4145

(-) for interrupted; (*) for disordered structures

Table S 2: Framework density of all structures after geometry optimization

		IZA	Our work		
		Silicates	Silicates	**Silicogermanates** (Ge in the full d4r)	**Aluminosilicates**
IZA Structural code	**N_{d4r}/N_T**	**Framework density (T/1000Å^3)**			
Regular					
ASV [1]	0.10	19.1	19.5	16.8	18.1
BEC [2-5]	0.06	15.1	14.9	13.7	14.6
IRN [6]	0.09	15.3	15.2	14.4	14.9
IRR [7-10]	0.06	11.8	11.6	10.7	10.9
ITG [11]	0.04	16.6	16.3	15.7	16.2
ITR [12,13]	0.04	17.4	17.2	16.6	17.2
ITT [14-20]	0.07	12.8	12.7	11.7	12.1
IWR [21-23]	0.04	15.6	15.4	14.8	15.1
IWS [24]	0.06	14.8	14.6	13.4	13.9
IWW [25-28]	0.04	16.6	16.4	15.8	16.2
POS [29]	0.06	15.5	15.3	14.2	14.7
SOF [30]	0.10	16.4	16.3	15.2	15.9
SOR [31,32]	0.08	17.1	16.9	15.7	17.6
SOV [33]	0.06	13.3	15.1	13.9	15.1
STW [30,34]	0.10	16.4	16	14.9	14.9
SVV [35,36]	0.04	18	17.8	17.6	17.7
UOS [37]	0.08	17.6	17.4	16.3	17.4
UOV [38]	0.03	16.2	16	15.6	15.9
UOZ [39]	0.10	19.5	19.3	17.4	18.1
UTL [40-43]	0.03	15.6	15.4	14.9	15.1
UWY [44]	0.05	16.3	16.2	15.3	15.9
Interrupted					
-IFT [45]	0.05	12.1	11.9	11.5	11.7
-IFU [46]	0.09	12.1	12	10.9	11
-IRY [47]	0.08	11.1	10.9	9.9	10.2
-ITV [8,48-50]	0.10	10.5	10.5	10.5	10.5
Partially Disordered					
***CTH [51-54]**	0.03	16.2	16	15.6	16.4
***UOE [55]**	0.08	17.6	17.4	16.4	18.3

(-) for interrupted. (*) for disordered structures

Table S 3: Energies of formation of silicogermanates and their silicate and aluminosilicates counterparts and energies of substitution of Ge for Si and Al following Figure 6.

	ΔE_{form} / T (kJ/mol)			ΔE_{sub}/ T (kJ/mol)								
	Si	**Si-Ge**	**Si-Al**	Ge→Si					Ge→Al			Si→Al
IZA Structural code	(full d4r)	(full d4r)	(full d4r)	Full Ge →Half Ge alternated	Full Ge →Half Ge in the s4r	Full Ge →Silicate	Half Ge alternated →Silicate	Half Ge in the s4r →Silicate	Full Ge →Aluminosilicate	Half Ge alternated → Aluminosilicate	Half Ge in the s4r → Aluminosilicate	Silicate → Aluminosilicate
Regular												
ASV [1]	13	50	21	-82.60	-84.22	-170.12	-87.51	-85.90	-183.93	-101.32	-99.71	-13.81
BEC [2-5]	14	37	19	-51.77	-54.43	-106.87	-55.10	-52.44	-114.66	-62.89	-60.23	-7.79
IRN [6]	14	47	21	-71.91	-75.59	-149.83	-77.92	-74.24	-160.89	-88.98	-85.30	-11.05
IRR [7-10]	17	36	21	-46.63	-45.68	-95.61	-48.99	-49.94	-103.85	-57.22	-58.17	-8.24
ITG [11]	12	23	14	-28.73	-29.23	-59.13	-30.40	-29.90	-65.14	-36.41	-35.91	-6.01
ITR [12,13]	11	24	14	-29.22	-30.17	-60.10	-30.88	-29.93	-65.11	-35.89	-34.94	-5.01
ITT [14-20]	16	35	21	-52.47	-51.52	-106.89	-54.42	-55.37	-115.57	-63.10	-64.05	-8.68
IWR [21-23]	13	24	15	-28.59	-29.55	-59.07	-30.48	-29.52	-64.21	-35.62	-34.66	-5.14
IWS [24]	14	35	19	-48.17	-49.16	-98.98	-50.81	-49.82	-106.67	-58.50	-57.51	-7.68
IWW [25-28]	12	24	16	-28.71	-29.63	-59.18	-30.48	-29.56	-62.90	-34.19	-33.27	-3.71
POS [29]	13	36	20	-51.05	-53.52	-105.94	-54.89	-52.42	-112.86	-61.81	-59.34	-6.92
SOF [30]	14	46	27	-80.19	-81.46	-165.35	-85.16	-83.89	-174.02	-93.83	-92.55	-8.66
SOR [31,32]	12	42	16	-69.41	-70.07	-141.07	-71.66	-71.00	-155.30	-85.89	-85.23	-14.23
SOV [33]	13	36	17	-51.31	-52.86	-106.07	-54.76	-53.22	-115.41	-64.10	-62.55	-9.34
STW [30,34]	15	48	24	-79.81	-81.90	-167.21	-87.40	-85.31	-179.27	-99.46	-97.37	-12.06
SVV [35,36]	11	23	13	-28.84	-29.40	-59.91	-31.07	-30.51	-65.51	-36.67	-36.11	-5.60
UOS [37]	12	40	18	-67.70	-68.35	-139.76	-72.06	-71.41	-150.80	-83.11	-82.46	-11.05
UOV [38]	13	24	15	-27.59	-28.24	-56.86	-29.27	-28.62	-61.47	-33.88	-33.23	-4.61
UOZ [39]	13	50	21	-84.72	-85.68	-170.80	-86.08	-85.12	-183.97	-99.24	-98.29	-13.16
UTL [40-43]	13	20	14	-20.81	-21.05	-42.95	-22.14	-21.90	-46.75	-25.94	-25.71	-3.81
UWY [44]	12	29	16	-40.78	-41.59	-84.02	-43.24	-42.43	-90.61	-49.83	-49.02	-6.59
Interrupted												
-IFT [45]	**17**	35	-14	-42.40	-42.71	-88.14	-45.74	-45.44	-94.43	-52.03	-51.72	-6.29
-IFU [46]	**14**	44	-21	-74.61	-75.84	-154.90	-80.29	-79.06	-166.96	-92.35	-91.12	-12.06
-IRY [47]	**18**	42	-13	-62.64	-62.62	-129.89	-67.25	-67.27	-140.92	-78.27	-78.29	-11.03
-ITV [8,48-50]	**15**	49	-89	-83.61	-85.62	-173.71	-90.10	-88.09	-185.54	-101.93	-99.92	-11.83
Partially Disordered												
***CTH [51-54]**	14	24	14	-27.29	-27.82	-51.39	-24.09	-23.57	-57.98	-30.69	-30.16	-6.59
***UOE [55]**	12	41	15	-67.59	-68.26	-139.76	-72.17	-71.50	-154.90	-87.31	-86.64	-15.13

(-) for interrupted. (*) for disordered structures

Table S 4: Gibbs free energies of substitution of Ge for Si ($\Delta G_{sub(1),\ Ge\rightarrow Si}$) and Ge for Al ($\Delta G_{sub(2),\ Ge\rightarrow Al}$) at different temperatures.

	$\Delta G_{sub(1),\ Ge\rightarrow Si}$			$\Delta G_{sub(2),\ Ge\rightarrow Al}$		
	Temperature (K)					
IZA Structural code	298	550	1000	298	550	1000
Regular						
ASV [1]	-53	-54	-56	-53	-44	-27
BEC [2-5]	-53	-54	-57	-53	-43	-26
IRN [6]	-53	-54	-56	-54	-44	-27
IRR [7-10]	-51	-53	-55	-52	-42	-25
ITG [11]	-51	-53	-55	-54	-44	-27
ITR [12,13]	-52	-53	-56	-53	-43	-26
ITT [14-20]	-51	-53	-55	-50	-41	-24
IWR [21-23]	-51	-52	-55	-52	-43	-26
IWS [24]	-52	-53	-56	-52	-43	-25
IWW [25-28]	-51	-53	-55	-50	-40	-23
POS [29]	-52	-53	-56	-52	-42	-25
SOF [30]	-51	-52	-55	-48	-39	-22
SOR [31,32]	-53	-54	-57	-52	-43	-26
SOV [33]	-52	-54	-56	-54	-45	-27
STW [30,34]	-51	-52	-55	-52	-43	-25
SVV [35,36]	-51	-53	-55	-54	-45	-27
UOS [37]	-52	-53	-56	-52	-43	-26
UOV [38]	-52	-53	-55	-52	-43	-25
UOZ [39]	-54	-55	-58	-52	-42	-25
UTL [40-43]	-50	-52	-54	-51	-42	-25
UWY [44]	-52	-53	-56	-52	-43	-26
Interrupted						
-IFT [45]	-51	-53	-55	-52	-42	-25
-IFU [46]	-51	-52	-55	-51	-42	-25
-IRY [47]	-51	-52	-54	-52	-42	-25
-ITV [8,48-50]	-51	-52	-55	-51	-42	-24
Partially Disordered						
***CTH [51-54]**	-56	-57	-59	-51	42	-25
***UOE [55]**	-52	-53	-56	-55	-46	-29

(-) for interrupted. (*) for disordered structures

Table S5: Si-O and Ge-O bond lengths (Å) computed for the BEC structure are various Si/Ge ratio.

Composition		**Average Si-O, Si out of d4r**	**Average Si-O, Si in d4r**	**Average Ge-O**
Silicate		1.618	1.624	-
Silicogermanate	Half occupation of d4r Ge in same s4r	1.620	1.624	1.778
	Half occupation of d4r Alternated	1.622	1.628	1.767
	Full occupation of d4r	1.625	-	1.774

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