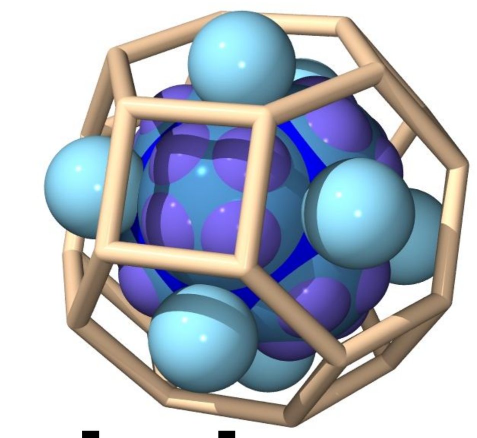

Towards an Atlas of Designer Zeolites – identification of unique topologies and Delaunay sphere analysis

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Introduction

- http://www.hypotheticalzeolites.net online since April 2004, contains approx. 5 million structures
- Receives ~10 visits per day
- A particular topology may be found repeated in different space sub-groups.
- Unique topologies have been identified using coordination sequences and vertex symbols
- Duplicate topologies can now be compared
- Delaunay sphere data analysis has been completed for all structures
- Additional tests confirming topology have been applied

Determination of topologically unique frameworks

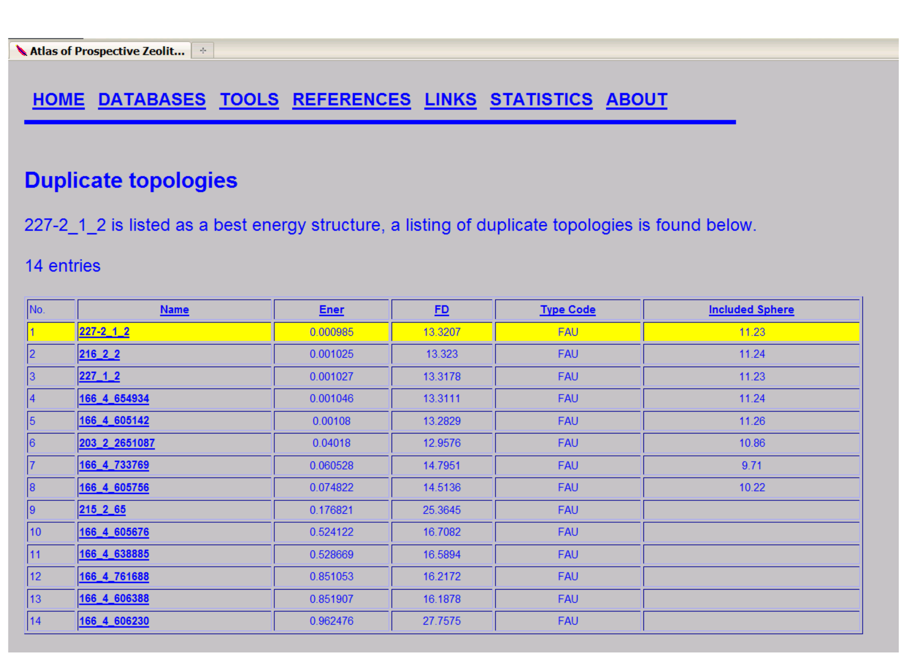
- Using coordination sequences (CS) and vertex symbols (VS) we have identified duplicate topologies
- The table below shows the number of structures for each *n*, the number of topologically equivalent T atoms

n	# of structures	# of unique topologies	# of structures < 0.1 eV/SiO_2*	# of unique topologies < 0.1 eV/SiO_2*
1	3870	526	759	90
2	80059	12556	11834	1111
3	105413	32429	10242	4202
4	825182	315908	42147	23420
5	4145644	1806970	110598	78612
6	229239	167127	15304	12538
Total	5389407	2335516	190884	119973

* Energy cutoff value is based on the BGB force field, relative to quartz as described in reference 2

Comparing duplicate topologies

Structures with the same topology can be listed and compared



This screenshot shows a listing of structures in the database with the FAU topology

Duplicate topologies

- Several topologies are found frequently
- In the table below we list the top 25 occurrences of topologies for structures generated with n = 1 & n = 2

n=1

	Structure	Type Code	Count	E	FD
1	19_2_1779	ABW	1301	0.00	22.4
2	19_1_4	cri	1244	0.00	23.7
3	70-2_2_386071		720	0.04	29.7
4	82_1_15	BCT	591	0.00	22.3
5	150_2_17892	tri	547	0.00	23.1
6	5_2_24374		507	0.00	26.8
7	91_2_8523379		410	0.70	33.3
8	2_2_652980		308	0.04	23.4
9	136_1_3	DFT	303	0.00	20.0
10	161_2_5322	SOD	262	0.00	19.2
11	13_2_253556		251	0.70	28.6
12	17_2_27747		250	0.58	30.1
13	145_1_30	qua	245	0.00	27.6
14	20_2_28244	NPO	242	0.00	18.3
15	66_2_3799	ACO	236	0.01	17.5
16	12_2_26630	ATN	175	0.00	21.1
17	50-2_2_16204		151	0.17	22.6
18	95_2_4735457		151	0.73	33.3
19	88-2_1_28	GIS	143	0.00	19.3
20	62_3_5917516		141	0.01	17.6
21	22_2_29178		131	0.07	9.2
22	84_2_713		116	0.00	21.4
23	2_2_419589		113	0.81	33.3
24	155_1_9		112	0.01	20.9
25	62_3_6071122	CAN	109	0.00	19.6

n=2

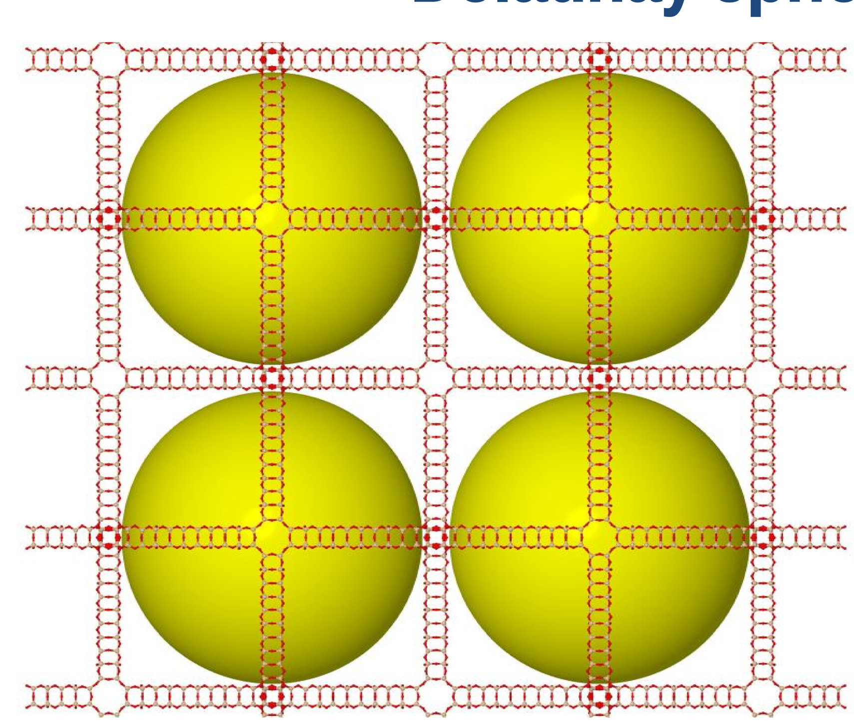
Structure	Type Code	Count	E	FD
2_2_23901		1866	0.86	26.2
14_2_42827		1106	0.13	25.9
2_2_558608		559	0.84	33.3
2_2_601528		482	0.39	29.6
60_2_23160		469	0.03	24.6
2_2_559953		309	0.87	32.7
61_3_13271556	JBW	210	0.00	20.9
2_2_416019		193	0.49	33.3
61_3_35496765		159	0.00	22.3
62_3_1842131		159	0.03	25.2
13_2_264168		120	0.05	23.9
15_2_196702		119	0.00	27.1
62_3_5872330		118	0.70	33.3
59_4_268633		116	0.03	12.8
74_3_2947490		114	0.01	19.8
69_3_40850		108	0.01	18.8
59_4_280211		106	0.23	25.7
2_2_624587		105	0.59	16.3
59_4_209724		105	0.04	20.4
49_2_3256		102	0.05	22.8
49_2_124		101	0.02	21.5
151_2_3611718		100	0.19	25.4
62_3_5926573		99	0.25	27.6
64_2_12188		98	0.00	22.9
62_3_1794192		97	0.14	30.2

Delaunay spheres

- It is now possible to search the entire database on calculated sphere properties as described in reference 5

  This allows filtering for the following properties:
  - the diameter of the largest possible included sphere
  - the diameter of the largest-free-sphere that can diffuse along, a, b, c, ab, bc or abc
- These provide a quick and elegant indication of the porosity of the framework. Caution is needed when comparing to molecular diffusion data.
- This data enables one to examine the nature of the framework i.e. cavities and channel dimensions without **looking** at the structure. This is useful for large databases.

Delaunay Sphere Example



The image shows the structure 229_5_489716, which has favorable energetics and a very low framework density. The calculated included-sphere and free-sphere diameters are among the largest found in the database so far, 58.7 Å and 36.8 Å respectively.

TOPOS confirmation of topological properties

- A subset of structures was analyzed by V. A. Blatov and D. M. Proserpio using the TOPOS program. http://www.topos.ssu.samara.ru/
- The majority of topologies were confirmed, providing an important data check.

Links to other databases

- Using the same technique for matching topologies based on CS & VS data, we have been able to link to other structures in other databases.
  - EPINET - http://epinet.anu.edu.au/
  - Structures generated by M.W. Deem and co-workers http://www.hypotheticalzeolites.net/DATABASE/DEEM/

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