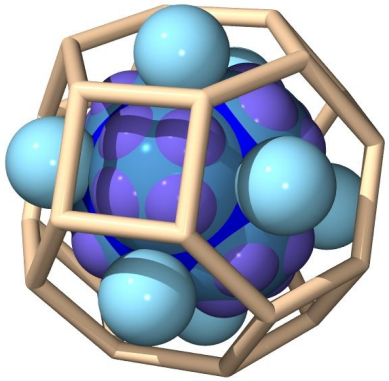

Progress towards an atlas of designer zeolites

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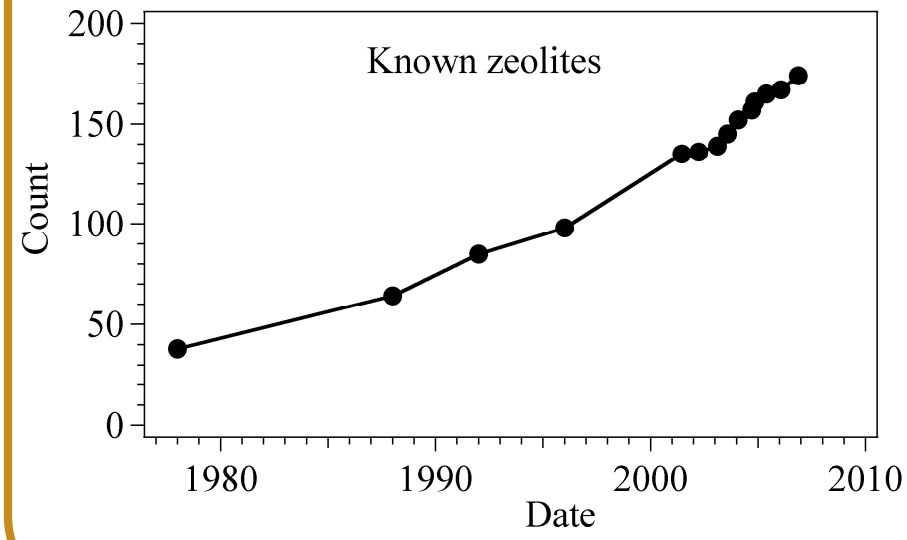
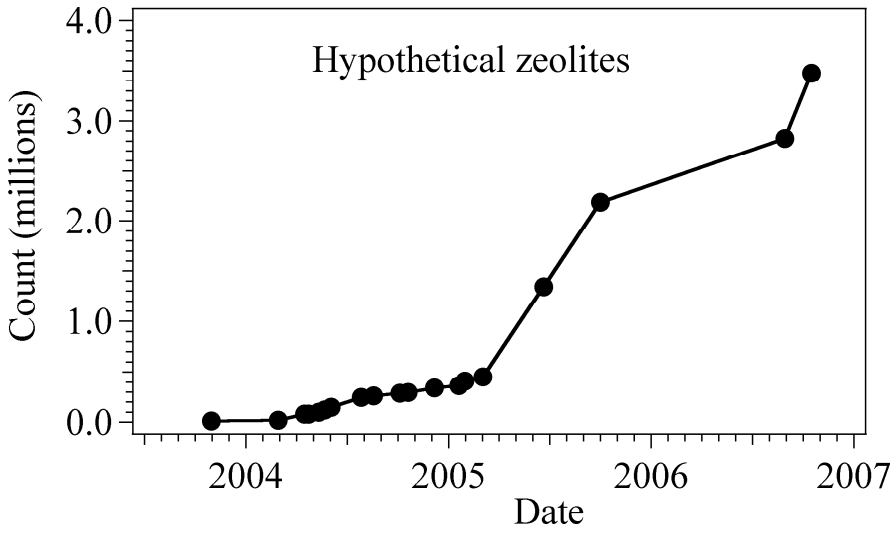
Introduction

- Collection of computer generated zeolite structures
- http://www.hypotheticalzeolites.net
- Online since April 2004, contains approx. 3 million structures.
- Receives ~10 visits per day

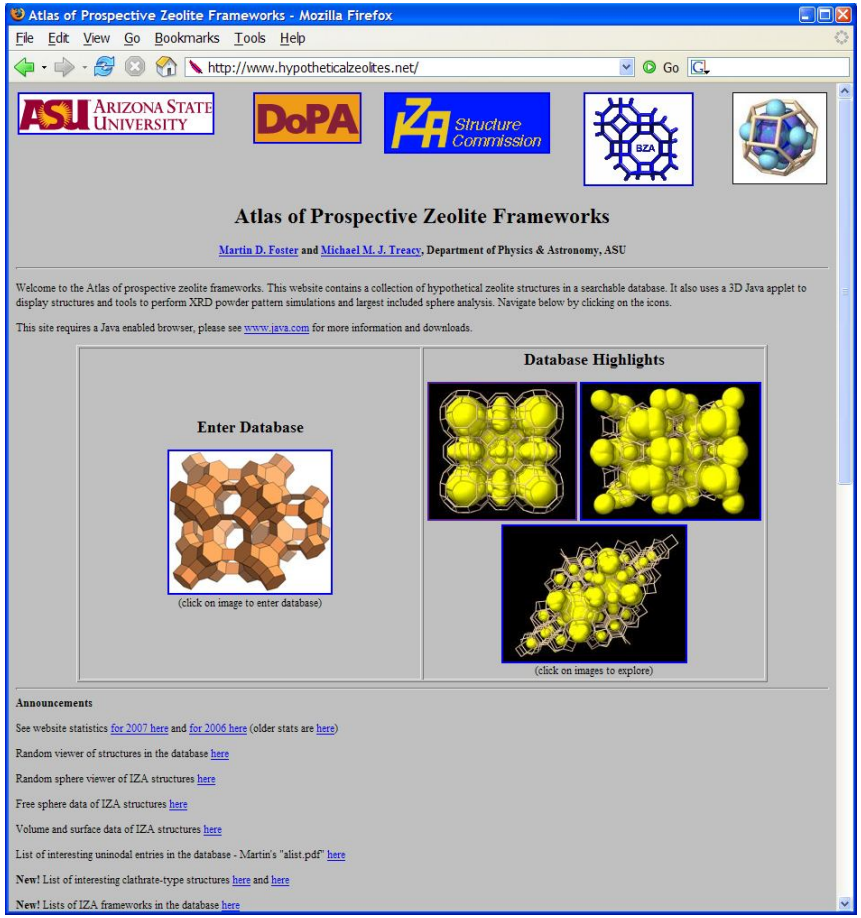


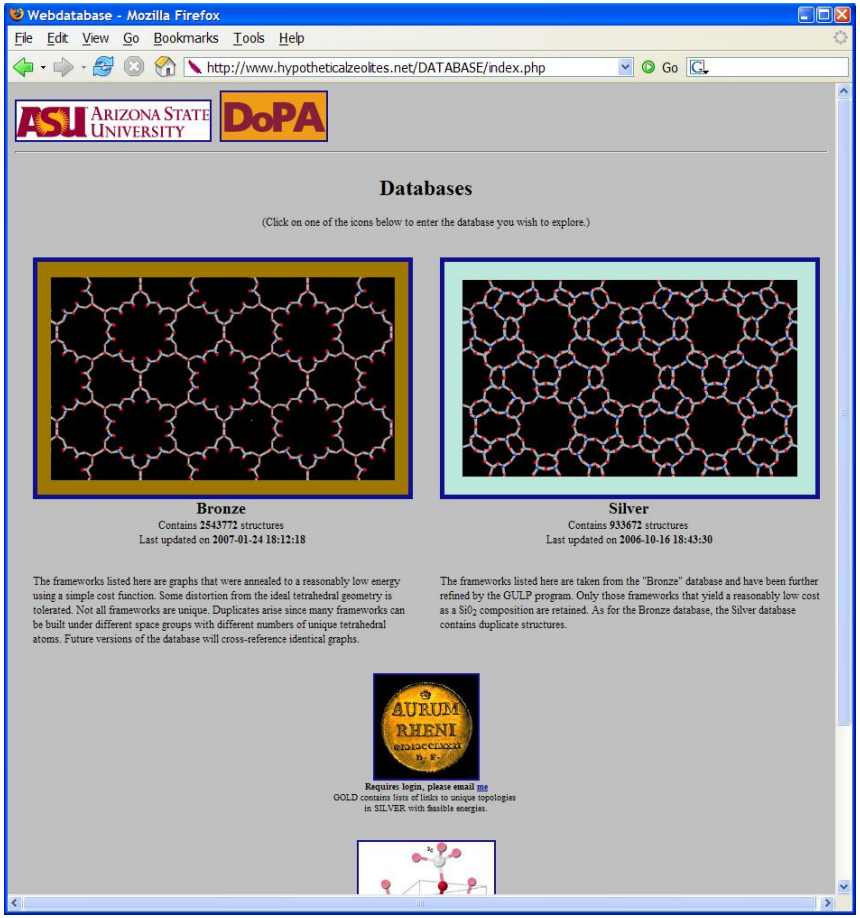


Website Objectives

- Provide online browsing of structures
  - 3D framework viewing
  - Download structure files (CIF files)
  - Tools to analyze structure
- Provide a search interface
  - Search structure listings for desirable properties
  - Find models for solving structures
- Provides a data set of structures for the discovery of new theories linking structure, topology, symmetry and inorganic chemistry

Website Contents





Database is split into sections demonstrating various levels of refinement, Bronze, Silver and Gold.

Bronze Contents

- Bronze structures are refined by TO_anneal which uses a modified forcefield for SiO_2 structures
- The energy is given in eV per SiO_2 unit relative to quartz
- Structures with a value of < 1 eV are retained in Bronze
- N = number of symmetrically equivalent T-atoms
- For n=1 and n=2, all graphs for all space groups have been computed and refined
- For n>2 selected space groups (productive) ones have been processed, e.g. space group 191 has been calculated up to n=6
- N=7 is our current technological limit

Silver Contents

- Structures in the Silver section are structures refined using SiO_2 interatomic potentials with the GULP program
- Structures in Bronze have an energy of 0.5 eV or lower
- GULP geometry optimisation is performed with symmetry enabled, however connectivity is not enforced
- Since we refine relatively good structures with GULP, only a small percentage will lose their original connectivity when refined with GULP
- We find a good agreement between the BGB cost function refinement and the GULP refinement.

Gold Contents

- Gold section contains lists of links to structures in Silver for n=1 and n=2 structures (< 0.3 eV GULP)
- The Gold structures have been filtered to contain only topologically unique structures in their lowest energy configuration – although highly dependent on space group, this listing provides a top level listing of very good structures
- Filtering the entire database has not been completed, but based on simple filtering techniques we estimate approximately 100,000 unique topologies

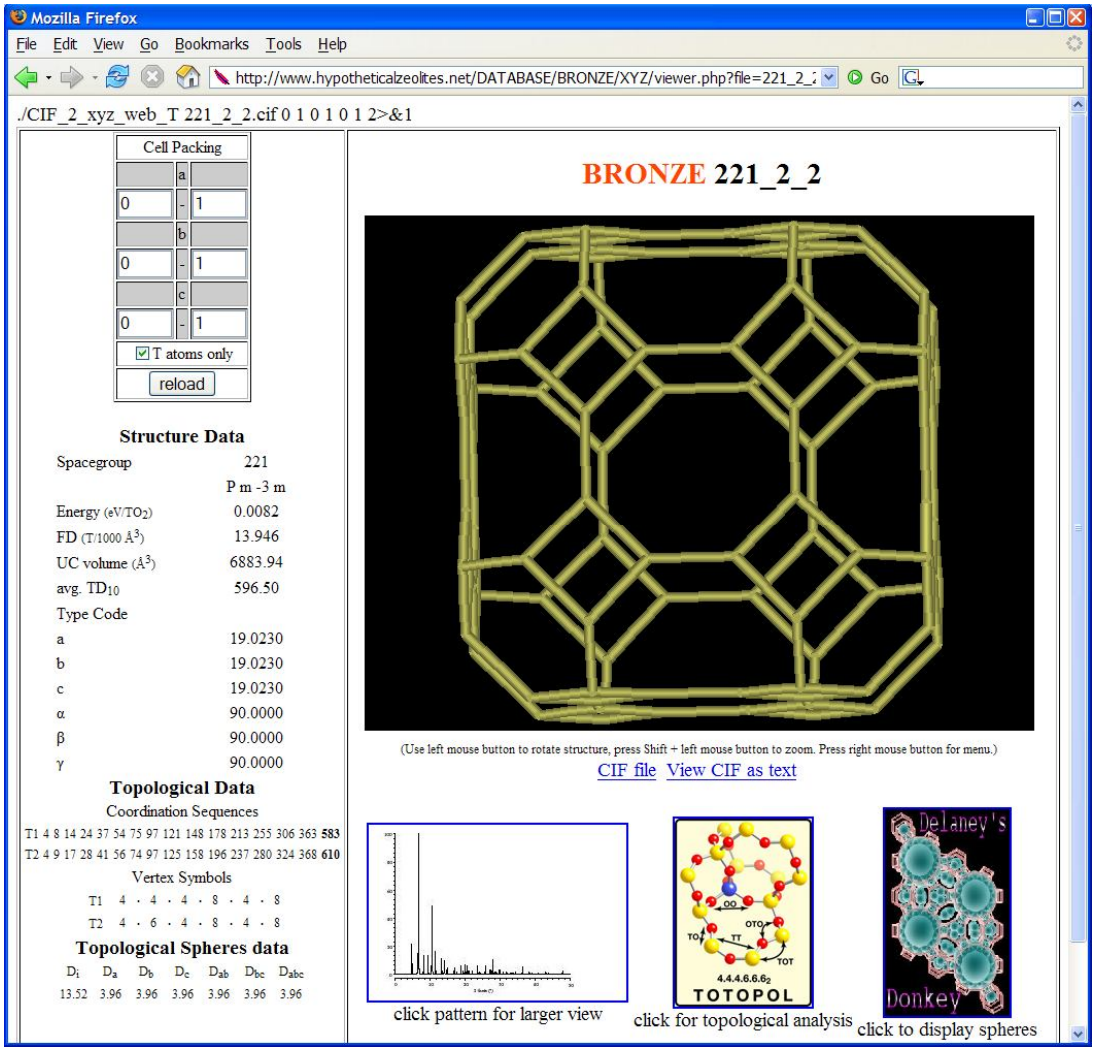
Searching the database

- Structures can be searched on a number of properties
  - Number of T atoms
  - Space group
  - Cell parameters
  - Framework density
  - Calculated energy
  - Largest included sphere
  - Smallest free sphere
- A web page where max and min values for the above parameters can be entered, acts as an interface for searching the database

Analysing Structures

Several programs are available to analyse a structure

- 3D viewer CIF viewer
- CIF_2_XRD – XRD powder pattern simulation
- TOTOPOL – topological analysis tool
- Delaney's Donkey – Sphere analysis tool

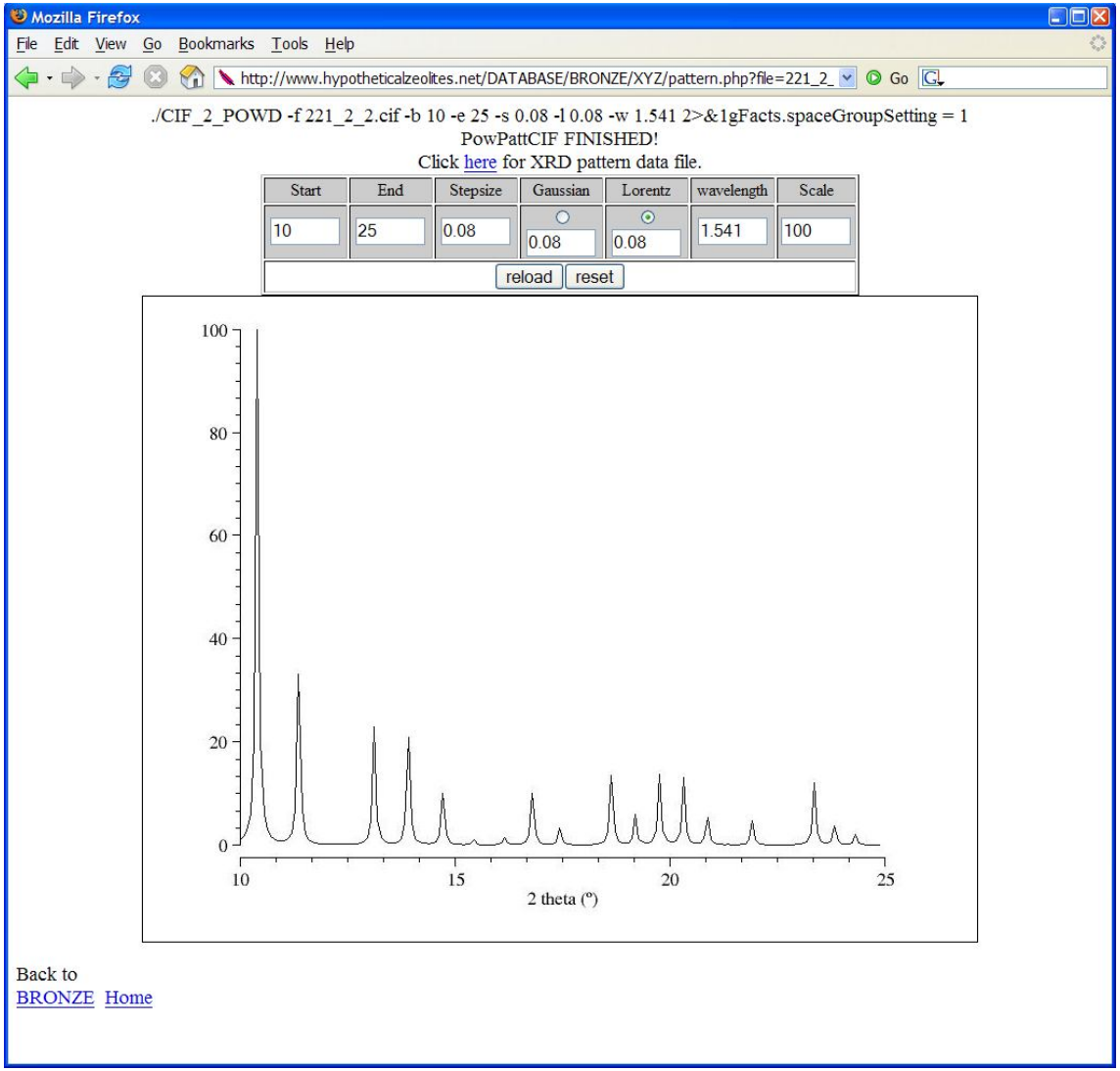


CIF_2_POWD

XRD powder simulation program

Variables which can be changed are

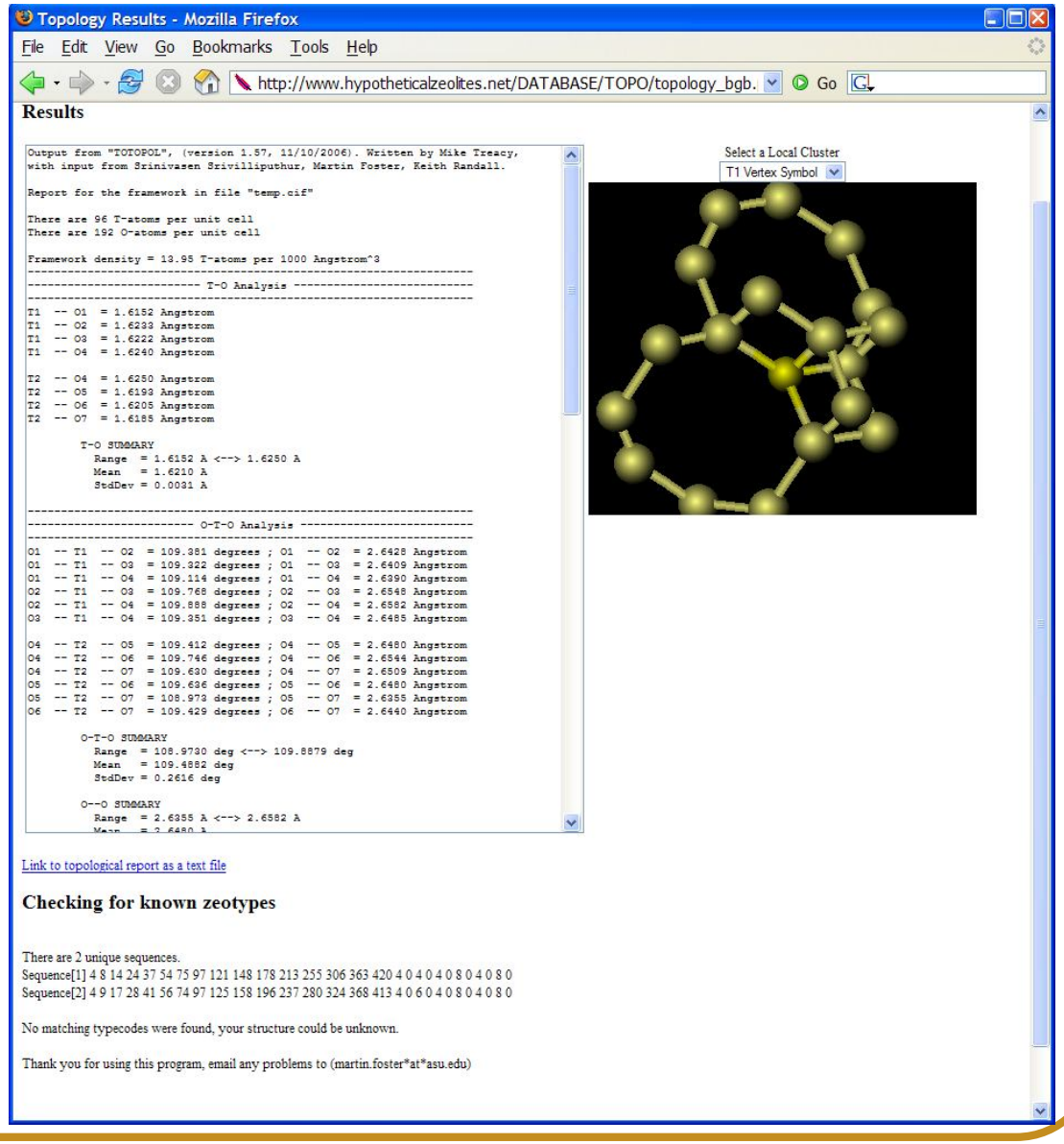
- Start & End points
- Step size
- Wavelength
- Scale



TOTOPOL

Topological analysis program calculates

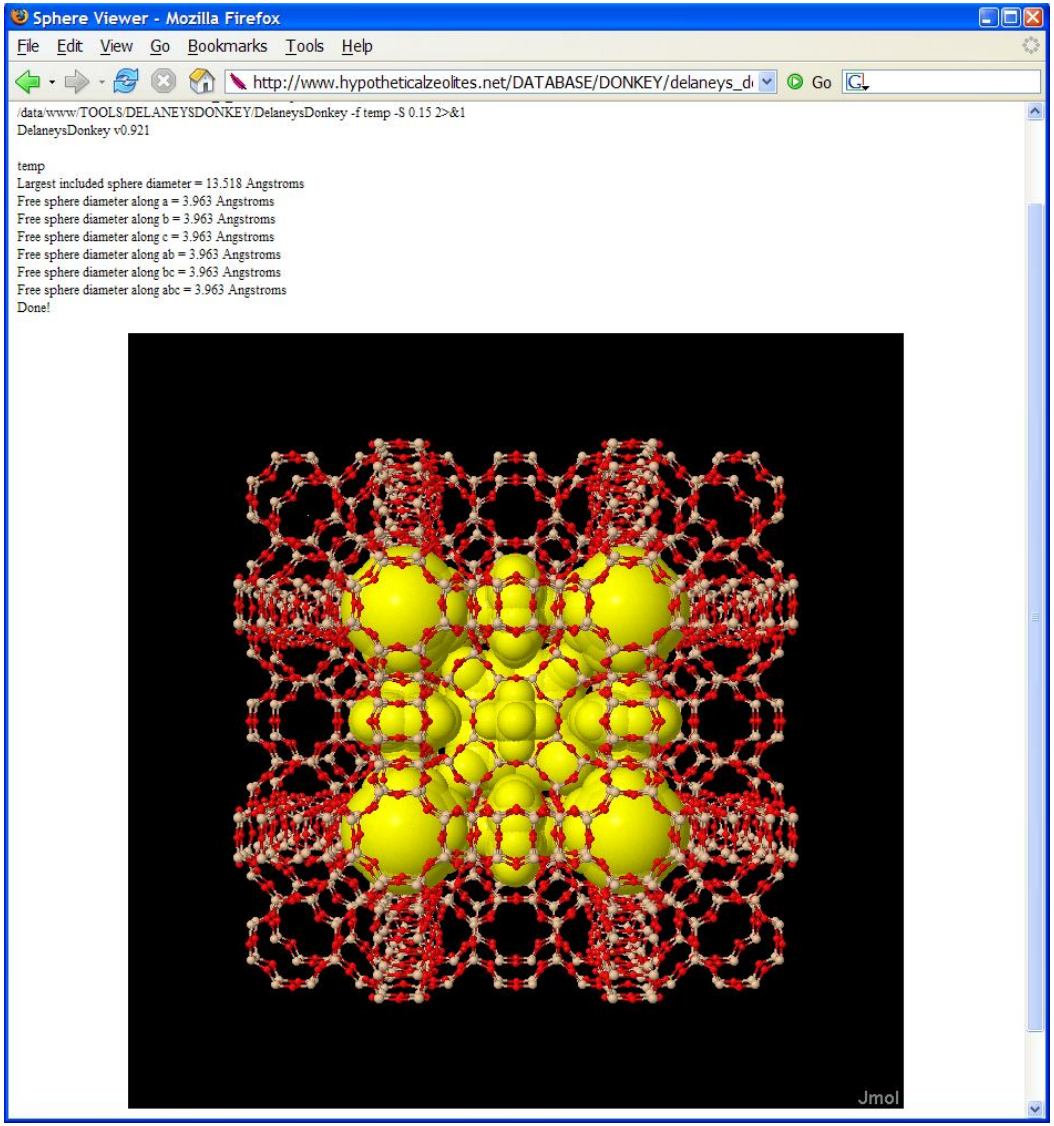
- Distances and angles
- Coordination sequences
- Circuit symbols
- Vertex symbols
- Topological check if a structure is a known IZA framework
- Statistical volume and surface calculation



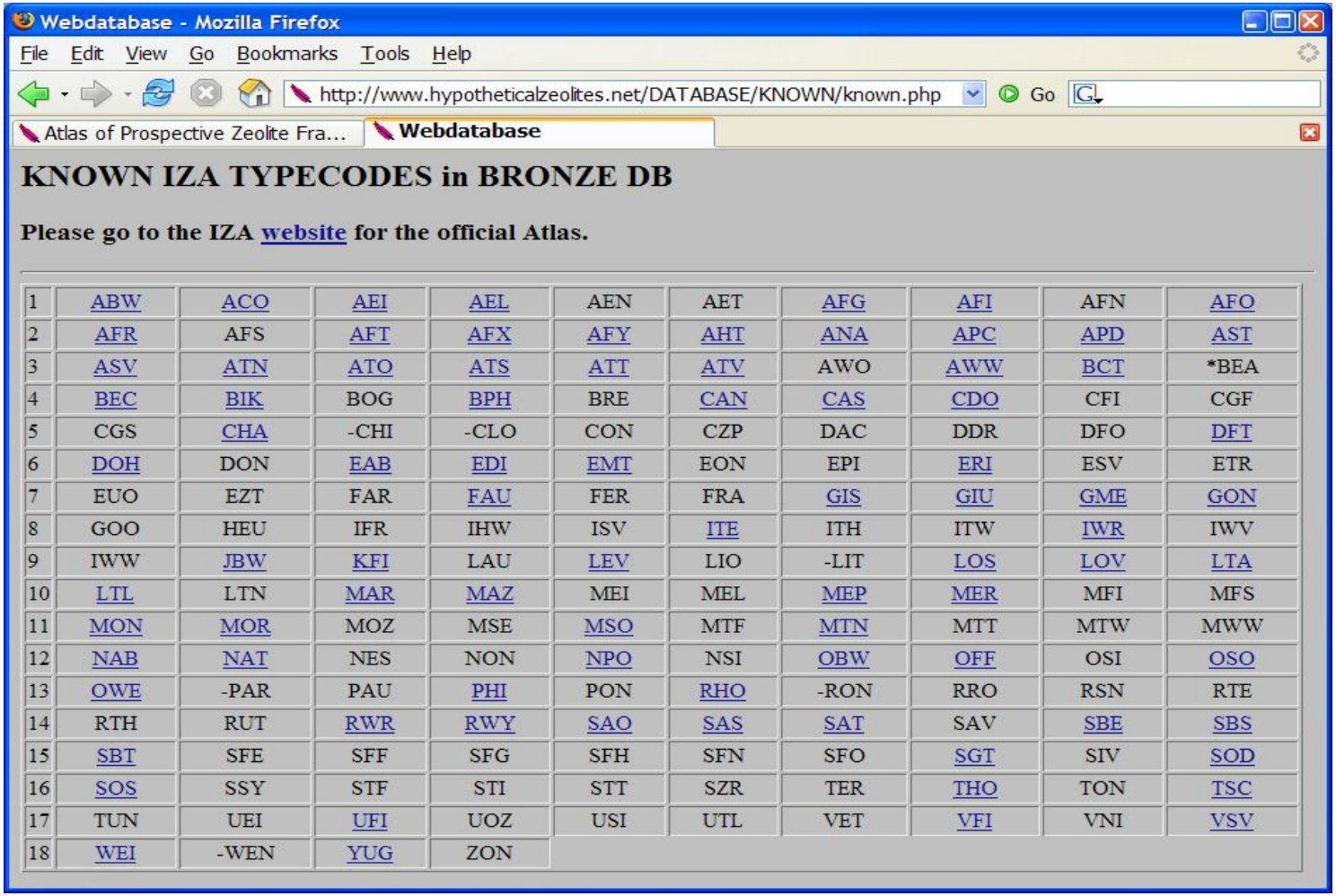
Sphere Analysis

Sphere Analysis calculates

- Largest included sphere
- Free sphere which passes through channel openings along a, b, c, ab, bc, and abc
- 3D viewer shows spheres in cavities and channels



IZA Structures found in the database



1	ABW	ACO	AEI	AEL	AEN	AET	AFG	AFI	AFN	AFO
2	AFR	AFS	AFT	AFX	AFY	AHT	ANA	APC	APD	AST
3	ASV	ATN	ATO	ATS	ATT	ATV	AWO	AWW	BCT	*BEA
4	BEC	BIK	BOG	BPH	BRE	CAN	CAS	CDO	CFI	CGF
5	CGS	CHA	-CHI	-CLO	CON	CZP	DAC	DDR	DFO	DFT
6	DOH	DON	EAB	EDI	EMT	EON	EPI	ERI	ESV	ETR
7	EUO	EZT	FAR	FAU	FER	FRA	GIS	GIU	GME	GON
8	GOO	HEU	IFR	IHW	ISV	ITE	ITH	ITW	IWR	IWV
9	IWW	JBW	KFI	LAU	LEV	LIO	-LIT	LOS	LOV	LTA
10	LTL	LTN	MAR	MAZ	MEI	MEL	MEP	MER	MFI	MFS
11	MON	MOR	MOZ	MSE	MSO	MTF	MTN	MTT	MTW	MWW
12	NAB	NAT	NES	NON	NPO	NSI	OBW	OFF	OSI	OSO
13	OWE	-PAR	PAU	PHI	PON	RHO	-RON	RRO	RSN	RTE
14	RTH	RUT	RWR	RWY	SAO	SAS	SAT	SAV	SBE	SBS
15	SBT	SFE	SFF	SFG	SFH	SFN	SFO	SGT	SIV	SOD
16	SOS	SSY	STF	STI	STT	SZR	TER	THO	TON	TSC
17	TUN	UEI	UFI	UOZ	USI	UTL	VET	VFI	VNI	VSV
18	WEI	-WEN	YUG	ZON						

3266 ABW 1308 BCT 307 SOD 265 DFT 227 ACO 205 NPO 175 ATN 158
GIS 82 MER 76 JBW 68 MON 67 CAN 64 CHA 58 RWY 58 RHO …

Conclusions

- Ultimately, the question is how far away are we from “designing” a zeolite structure and rational synthesis?
- Still far, but we show computationally that we can generate and refine a large number of zeolite structures and filter them into lists of desirable structures.
- We are making progress towards one of the hardest problems, creating an Atlas of feasible designer zeolites by Filtering for synthetic targets. These filters require understanding of fundamental questions in zeolite science, such as what makes a structure crystallize to the structure it does and why only a handful for topologies exist compared to the vast number of possibilities?
- We have shown the database to be useful for several applications such as confirming the ZSM-10 structure.
- We have shown that known IZA structure codes are found in a large number of space groups

References

1. M. M. J. Treacy, K. H Randall, S. Rao, J. A. Perry and D. J. Chadi, *Zeit. Krist.* 212, 768-791 (1997).
2. M. M. J. Treacy, I. Rivin, E. Balkovsky, K. H. Randall, and M. D. Foster. *Micropor. Mesopor. Mat*., 74(1-3):121–132, 2004.

Acknowledgments

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