How Worldwide is the Virtual Museum of Minerals and Molecules?

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Introduction

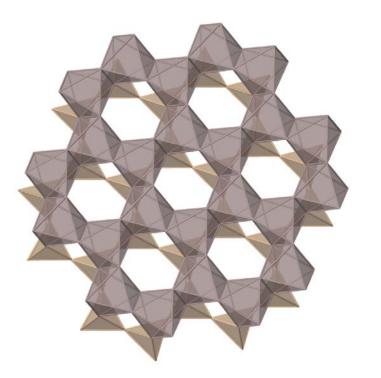
Initially funded by a UW-Madison Chancellor's Instructional Technology Grant in 1997, The Virtual Museum of Minerals and Molecules (VMMM) went live in 1998, and is active to the present. The goal was to put 3D molecular visualizations of minerals and molecules into the hands of students and instructors at the UW-Madison and the world through the relatively new medium of the world wide web.

https://virtual-museum.soils.wisc.edu

The VMMM is a web-based resource presenting 3D molecular visualizations of minerals and molecules of interest to soil and environmental sciences. The displays allow user manipulation of the visualizations, including transition from ball-and-stick mode to polyhedral representation and highlighting of specific structural features.

Objectives and Methods

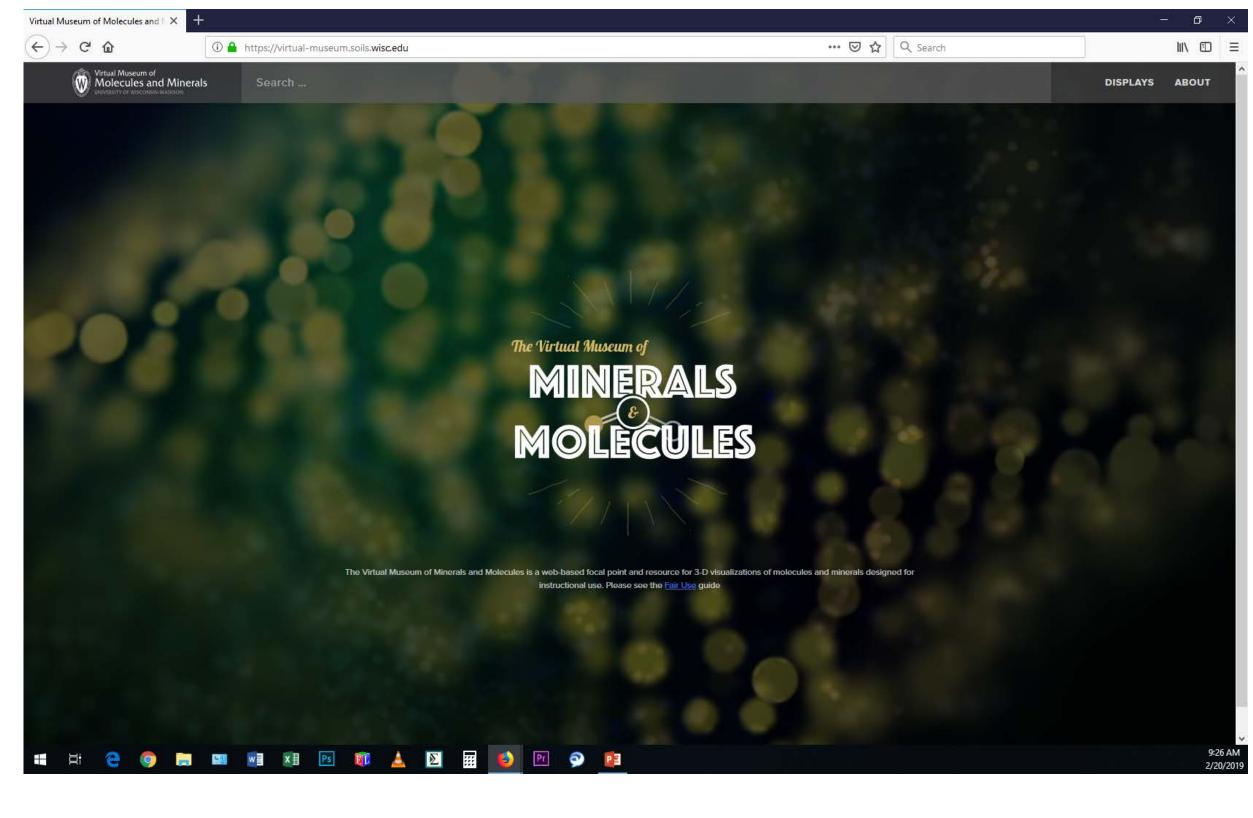
VMMM displays are used extensively in soil science courses at the UW-Madison for 21 years. Despite the absence of a formal dissemination plan, the VMMM ranks high in search engine listings. Curious about the greater body of users, Google Analytics was embedded into the latest version to track usage, starting in December 2016.



Discussion

Technologies to deliver the VMMM content on the web have changed over 21 years:

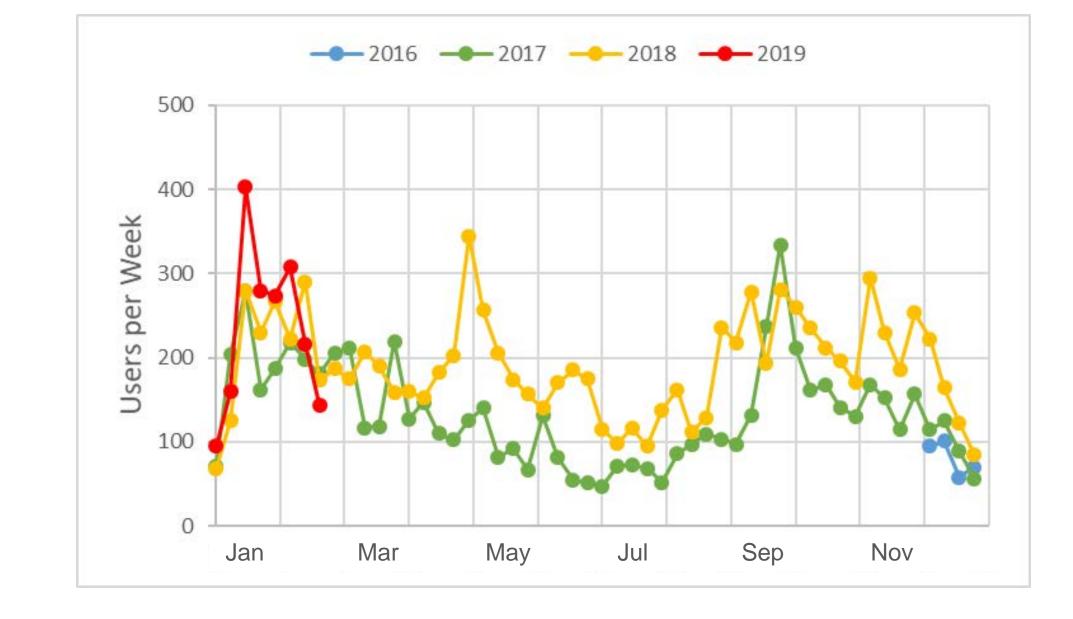
- Originally conceived in VRML (Virtual Reality Modeling Language), the VMMM launched in 1998 using a Chime plugin for Netscape and Safari.
- As Chime support dwindled, the Jmol open source community evolved to formulate a replacement based the ubiquitous Java plugin that all major browsers supported--"Write once, run everywhere". VMMM contributed bonding rules and polyhedral mode to Jmol.



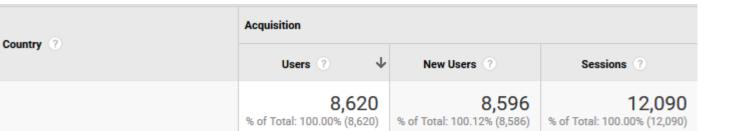
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Virtual Museum of Molecules and Miner	als	Search		DISPLAYS	ABOUT	^

Results

Data for 2018 show that the VMMM averaged ~1000 unique sessions per month, up 42% from 2017, and closely following the academic calendar. Pages per session average 6.4 and users average 3 minutes per session.



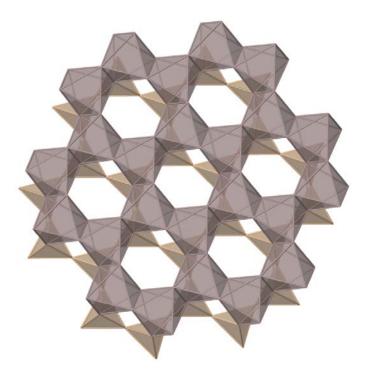
More than half of users are international, with 44% of sessions originating in the US and 3% from Wisconsin, including Madison.



- In 2005, the VMMM moved from Chime to Jmol, with an XML codebase.
- With increasing security issues with Java, browsers began to abandon Java and with it, Jmol and the VMMM. The Jmol community responded by recasting Jmol in javascript to create JSmol.
- In 2016, the VMMM was reformulated to use JSmol, with a WordPress template to make writing displays uniform.

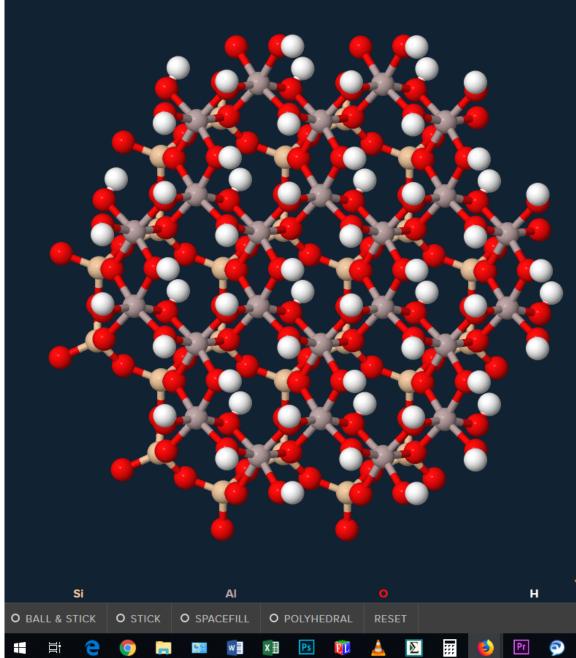
In addition to early financial support from the UW-Madison and the University of Minnesota, Twin Cities, the VMMM was twice funded by the USDA Higher Education Challenge Grant program, in 1998 for VMMM v1 and in 2004 for VMMM v2.

Over the years, a "wish list" of additional displays and features has accumulated, as well as some residual cleanup from the last reformulation, all pending further support.



Conclusions

With a relatively modest investment in educational innovation in 1997, the UW-Madison has been home to a learning tool that serves not only students in own classrooms but also students and instructors around the world, for 21 years.



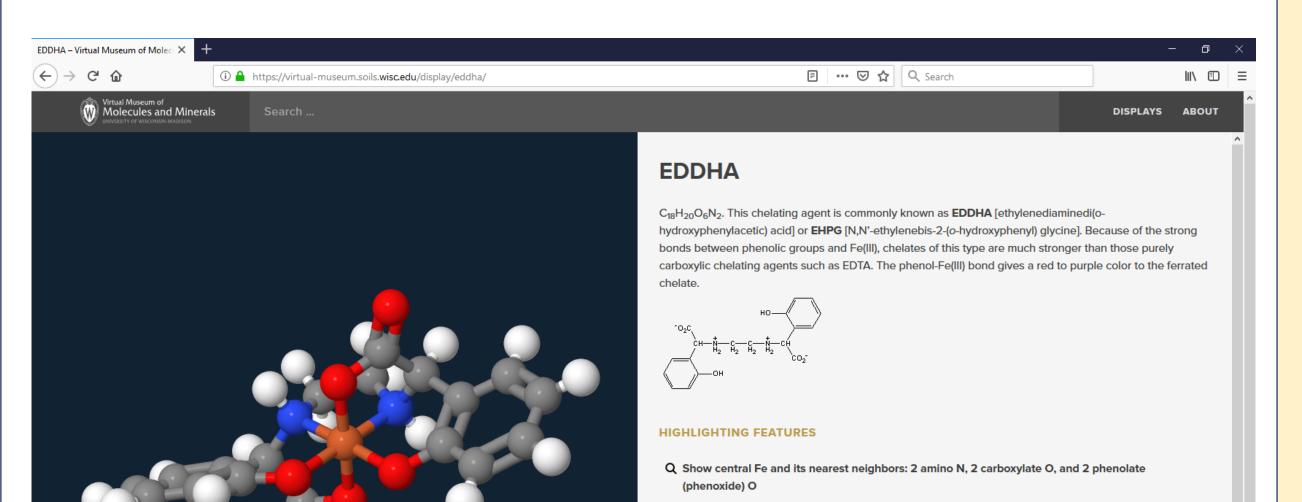
Kaolinite

Kaolinite is a common 1:1 dioctahedral phyllosilicate (clay) mineral found in soils across the world, particularly in highly-weathered environments, as well as scattered monomineralic deposits that are mined for industry. Being a 1:1 mineral, each kaolinite layer has one silica tetrahedral sheet and one alumina octahedral sheet. Individual layers are held together in a crystal by O - H - O bonds between the octahedral sheet of one layer and the tetrahedral sheet of the adjacent layer.

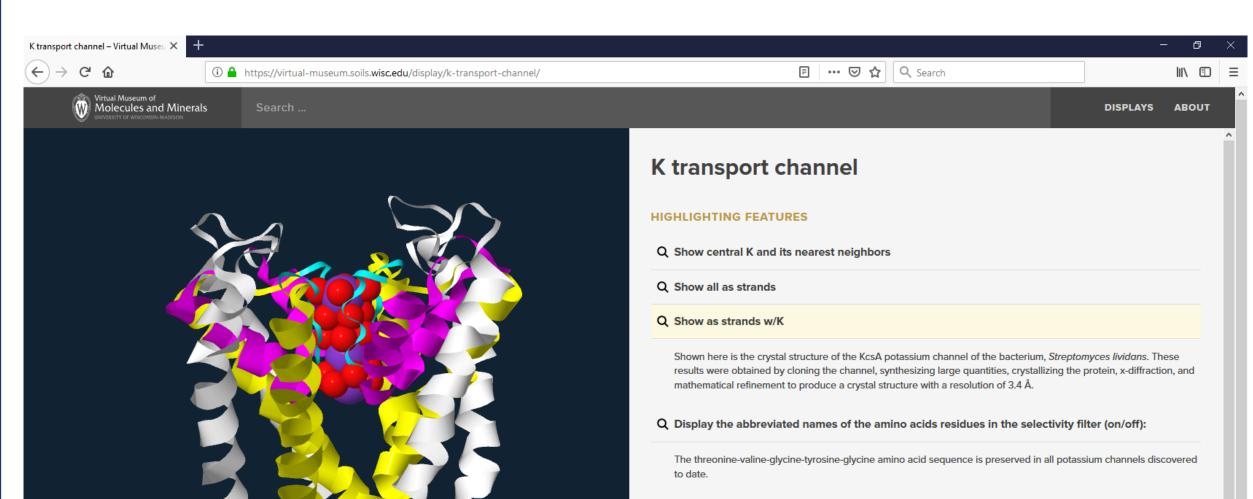
The crystallography of kaolinite played an important role in Linus Pauling's formulation of the nature of the chemical bond, although for 15 years kaolinite was thought to be monoclinic (crystallographic axes all equal to 90°) instead of triclinic. Crystallographic axes: alpha, 91.8°; beta 104.7°; gamma, 90°).

The crystal structure displayed to the left, including all H atoms, is based on low-temperature (1.5° K) neutron powder diffraction data (Bish, 1993) instead of the more common x-ray diffraction data that has been used since the time of Linus Pauling's original determination of the crystal structure of kaolinite in 1930.

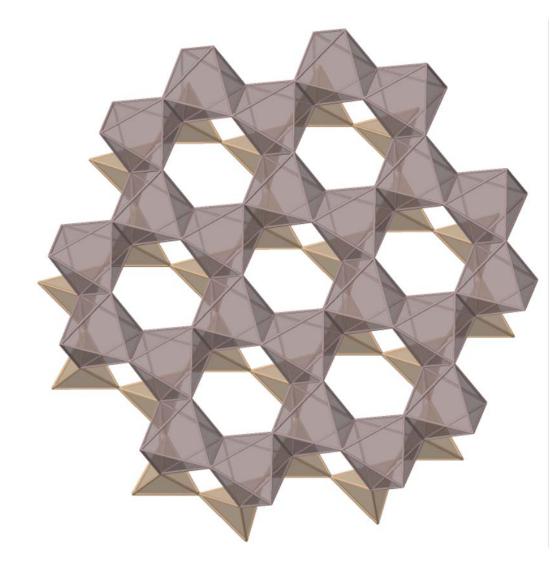
	HIGHLIGHTING FEATURES
	Q Plane of Si atoms
	Q Single silica tetrahedron
	Q Silica tetrahedral sheet
	Q Plane of Al atoms
	Q Single alumina octahedron
	Q Alumina octahedral sheet
JSmol	Q Single unit cell
	Q Show all atoms
P	<i>🦚</i>



		(0,000)				
1. 🗮 United States	3,828 (44.24%)	3,814 (44.37%)	4,954 (40.98%)			
2. 🔛 Australia	476 (5.50%)	474 (5.51%)	1,124 (9.30%)			
3. France	383 (4.43%)	355 (4.13%)	631 (5.22%)			
4. 🔚 India	378 (4.37%)	380 (4.42%)	433 (3.58%)			
5. 🚘 Colombia	247 (2.85%)	245 (2.85%)	453 (3.75%)			
6. 🕒 Canada	229 (2.65%)	228 (2.65%)	286 (2.37%)			
7. 鄙뚫 United Kingdom	206 (2.38%)	206 (2.4	Acquisition			
8. 🔯 Brazil	194 (2.24%)	193 (2.2	Kegion (Users ?	New Users ?	Sessions ?
9. 🚾 Spain	192 (2.22%)	191 (2.2		3,828	3,814	4,954
10. 📧 South Korea	172 (1.99%)	174 (2.0		% of Total: 44.41% (8,620)	% of Total: 44.42% (8,586)	% of Total: 40.98% (12,090)
		1	. California	488 (12.66%)	485 (12.72%)	586 (11.83%)
		2	. Ohio	338 (8.77%)	334 (8.76%)	389 (7.85%)
		3	New York	229 (5.94%)	227 (5.95%)	294 (5.93%)
		4	Wisconsin	184 (4.77%)	179 (4.69%)	252 (5.09%)
		5	Texas	178 (4.62%)	176 (4.61%)	251 (5.07%)
		6	. Pennsylvania	168 (4.36%)	166 (4.35%)	244 (4.93%)
		7	. (not set)	167 (4.33%)	165 (4.33%)	169 (3.41%)
		8	. Arizona	148 (3.84%)	148 (3.88%)	197 (3.98%)
		9	. Nebraska	142 (3.68%)	142 (3.72%)	161 (3.25%)
		10	Massachusetts	116 (3.01%)	115 (3.02%)	182 (3.67%)



Experience teaches that all such innovations require technology refreshes to avoid obsolescence and such maintenance should be considered at start up and on a continuing basis.



Acknowledgements

Many thanks to Al Nemec and Jason Pursian of CALS IT for carrying the VMMM into its latest incarnation, Yishai Barak for converting VMMM v2 into v3, CALS and the Dept of Soil Science for hosting the VMMM with a

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This model shows the near-perfect octahedral coordination of the central Fe atom, with two carboxylate oxygens, two phenolate oxygens, and two amino nitrogens as the apices of the octahedron. The symmetry of the central Fe atom with its nearest neighbors is a key factor in chelate stability.

In spacefilling mode, this model shows that the central Fe atom is nearly completely concealed by coordinating oxygens and nitrogens. No coordination by additional water (H₂O) or hydroxide (OH⁻) is permitted in this structure, a situation which adds to the stability of this chelate.

 Q ethylenediamine (H2NCH2CH2NH2)

 Q phenol [x2] (C6H6OH)

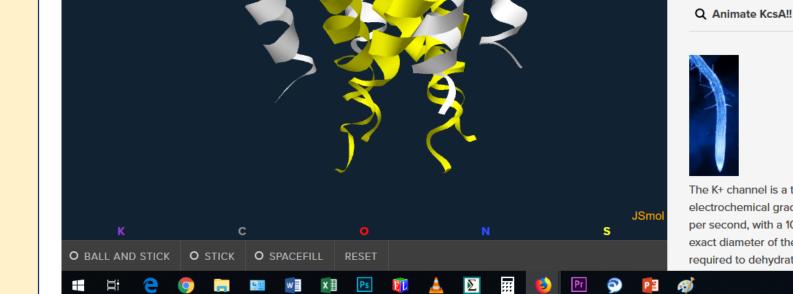
 JSmol

 Q acetic acid [x2] (CH2COOH)

 Q glycine [x2] (NH2CH2COOH)

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O BALL AND STICK O STICK O SPACEFILL RESET



The K+ channel is a transmembrane protein that permits the movement of K+ according to its electrochemical gradient from the outside of the cell to the cytoplasm. Throughput rates are up to 108 ions per second, with a 10 4:1 preference for K+ over Na+. The high selectivity for K + is dependent upon the exact diameter of the the selectivity filter, which exploits the difference between K+ and Na+ in the energy required to dehydrate the ion (which is inversely dependent upon the radius of the dehydrated ion) as it stable URL for these many years.

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