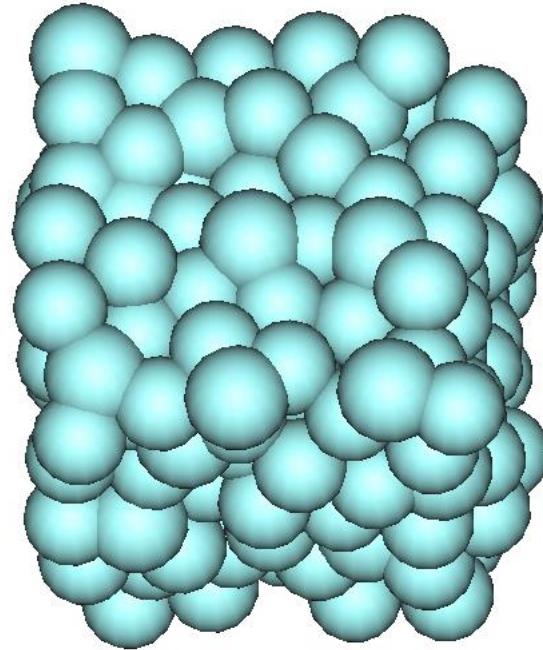


Geometry of molecules





**MOLECULAR GEOMETRY
AND
ITS APPLICATION TO
NANO INFORMATICS AND MOLECULAR DESIGN**

Sep 29, 2014

**The 11th Korea-U.S. Forum on Nanotechnology:
Nanomanufacturing, Nanocomposites and
Nanoinformatics
Seoul National University, Seoul, Korea**

Deok-Soo Kim

**Voronoi Diagram Research Center
School of Mechanical Engineering
Hanyang University, Seoul, Korea**

Molecular Structure/Function

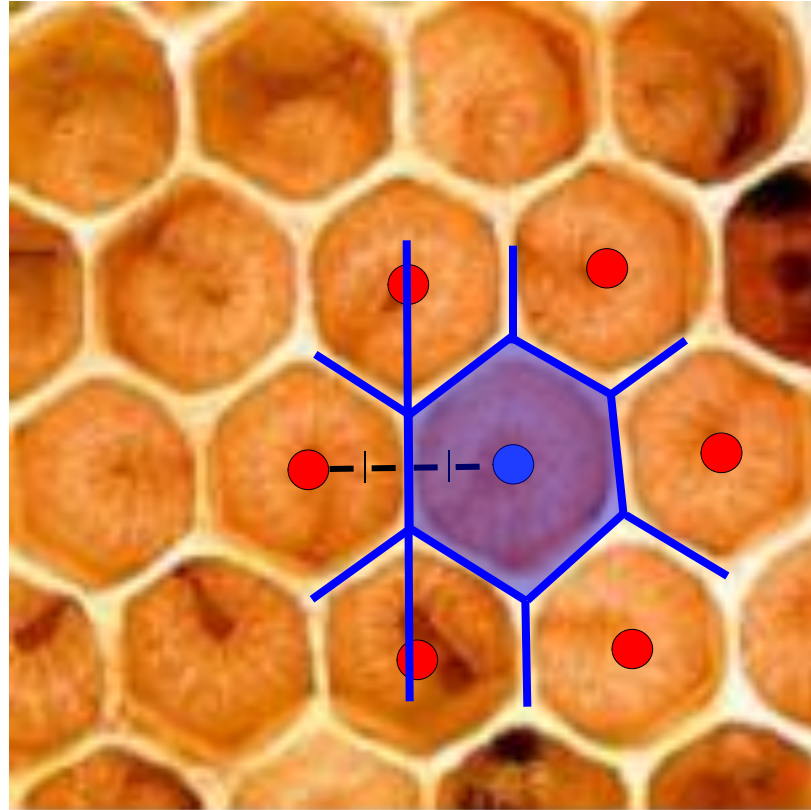
- **Structure Determines Function.**
- **Geometry Determines Structure.**
- **Organic and Inorganic...**
- **No Theory/Tool Yet.**

Contents

- **Voronoi Diagram +**
- **Applications**
- **MG (Molecular Geometry) and
MGOS (MG Operating System)**

VORONOI DIAGRAM

Voronoi Diagrams in Nature

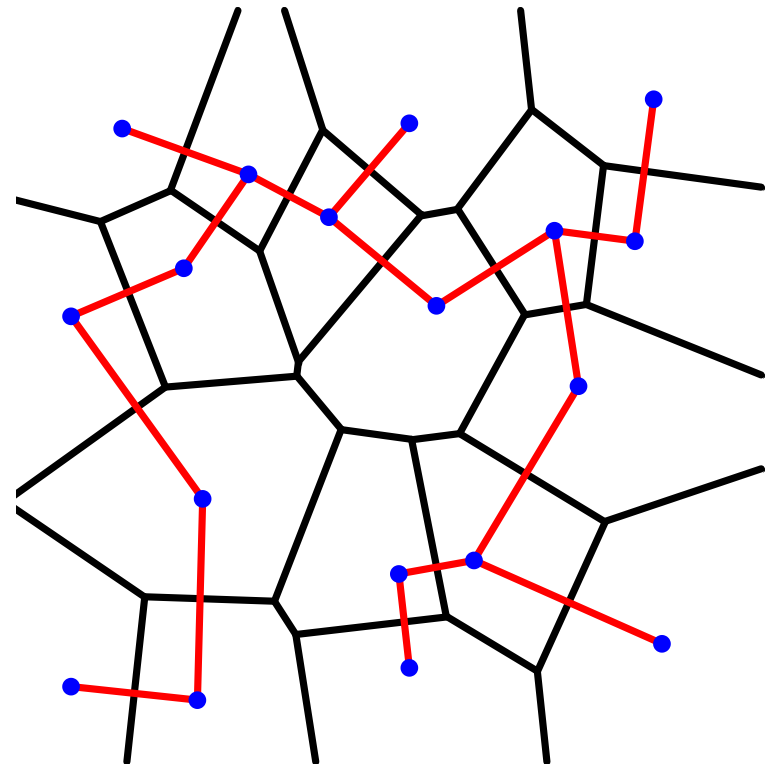


Wall : the edge of Voronoi Diagram

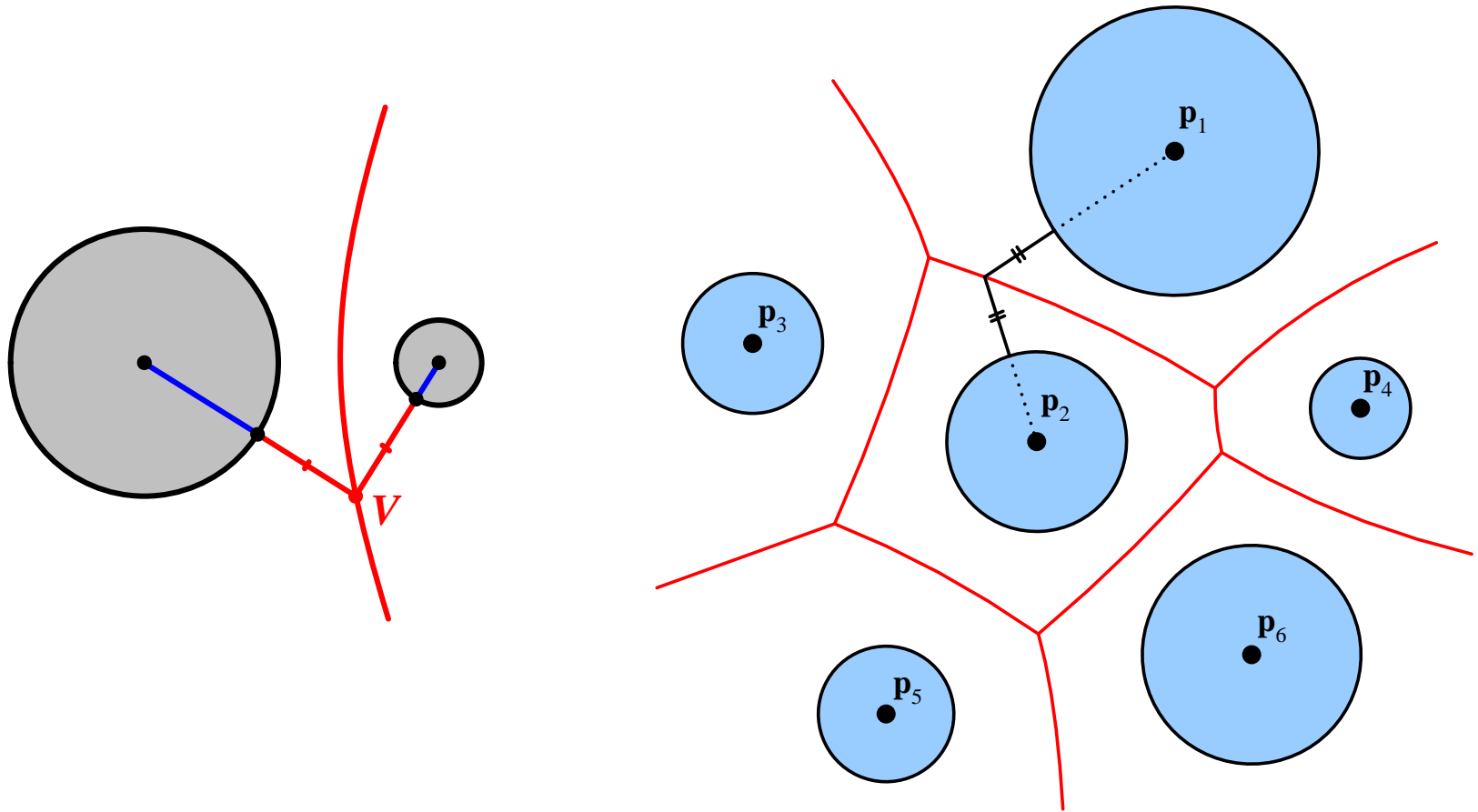
Cell : the Voronoi Region

Easily Solved Problems Using VD(P)

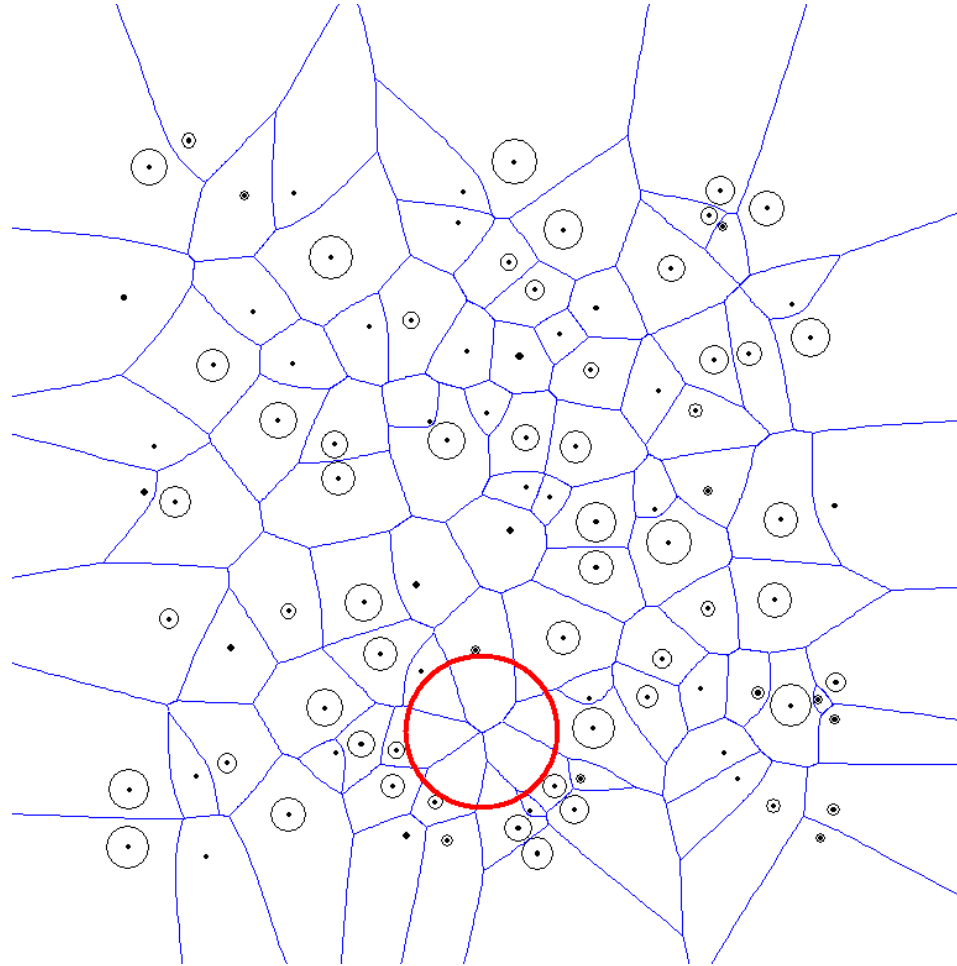
- Convex hull
- Largest empty circle
- Delaunay triangulation
- **Minimum spanning tree**
- Nearest neighbor
- Closest pair
- Etc.



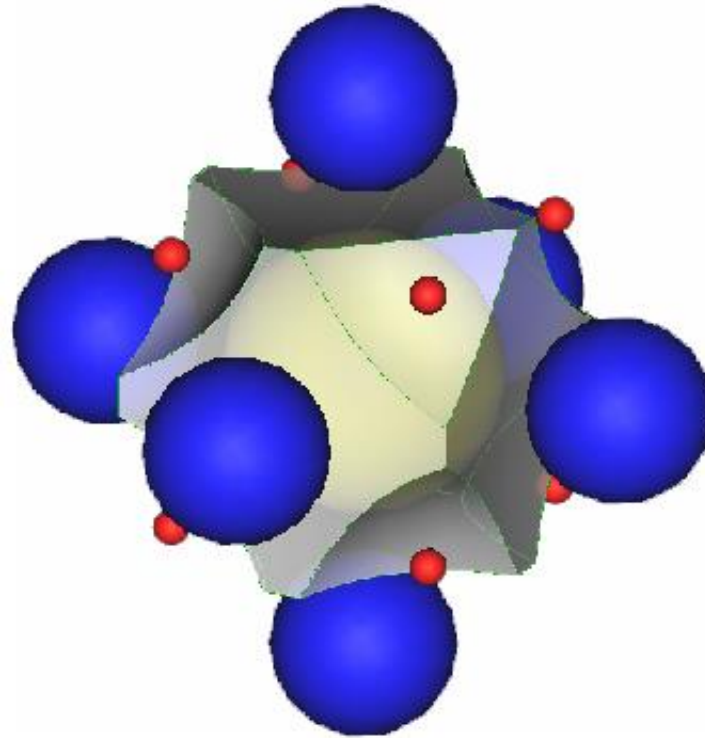
Voronoi Diagram of Circles (Additively-weighted VD)



Applications of VD(C)

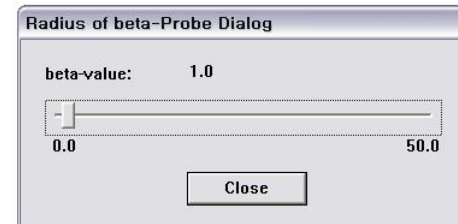
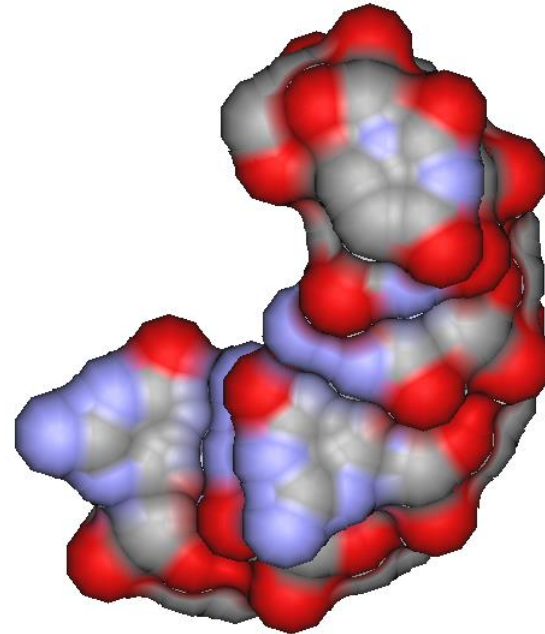
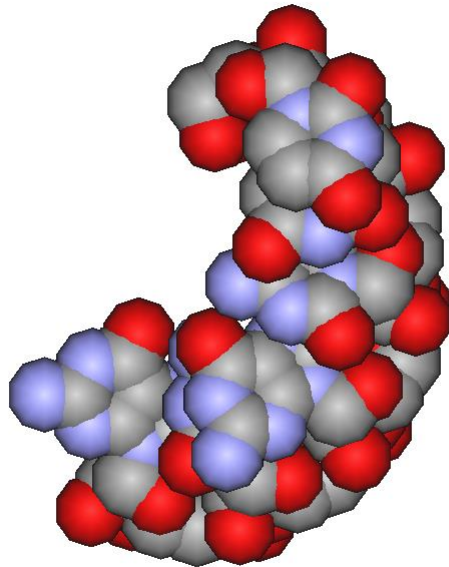


Voronoi Diagram of Spheres (Additively-weighted VD)



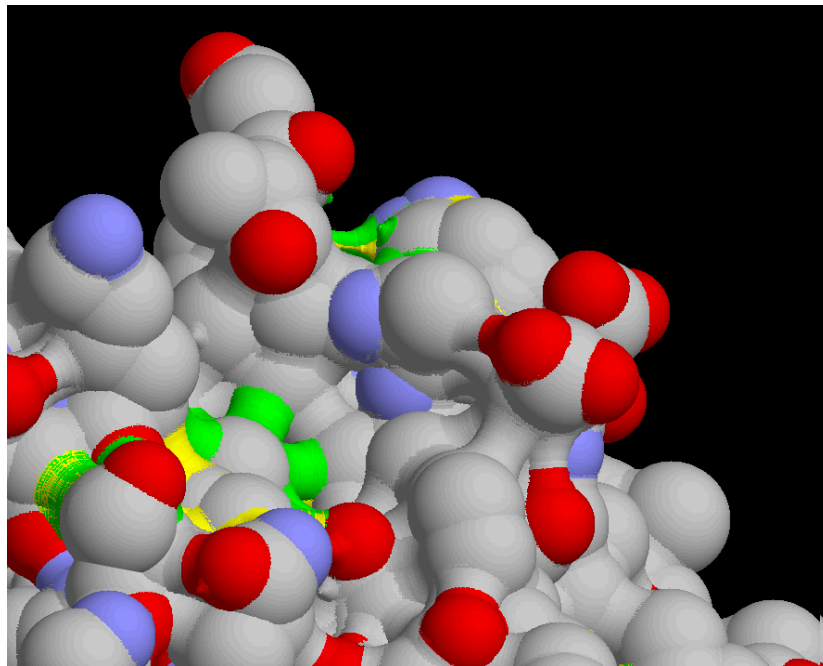
APPLICATIONS

Connolly Surface

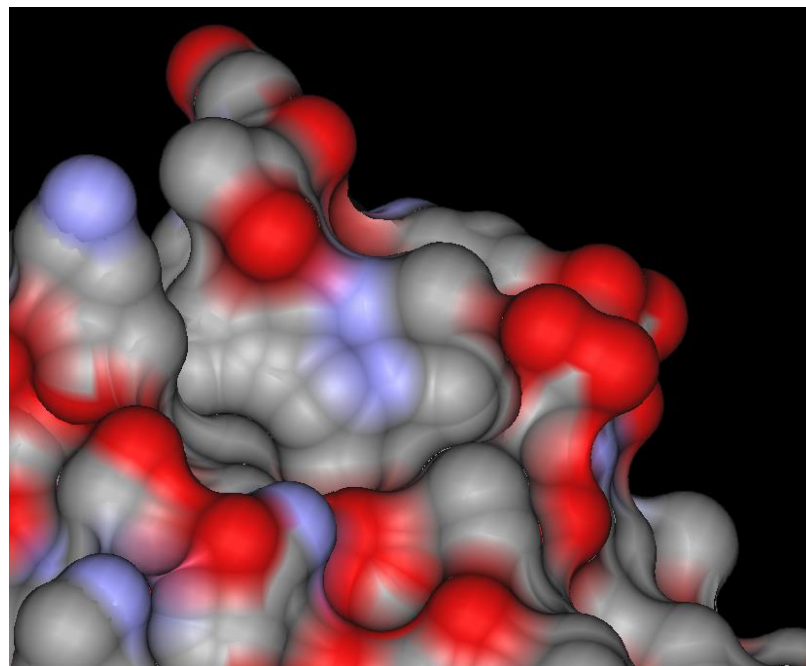


(Pentium IV, 3.2 GHz, 1 GB RAM)
(10us; Realtime computation and visualization)

Comparison: RasMol vs. BetaMol

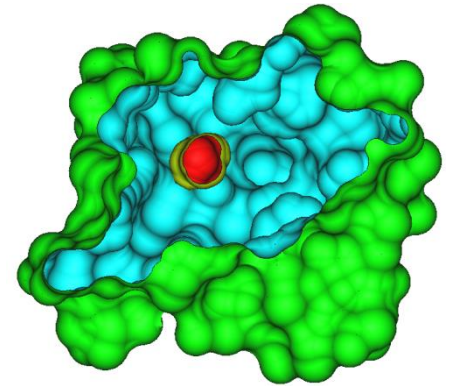
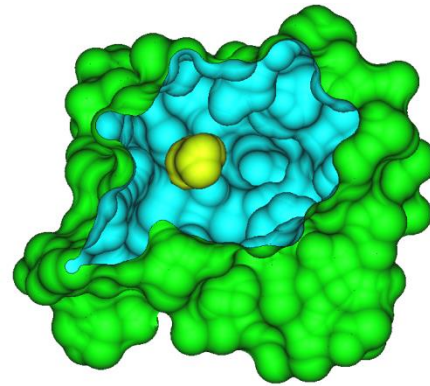
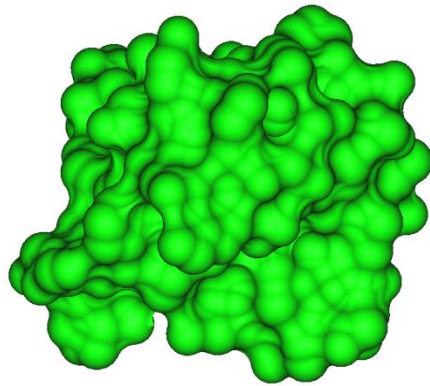
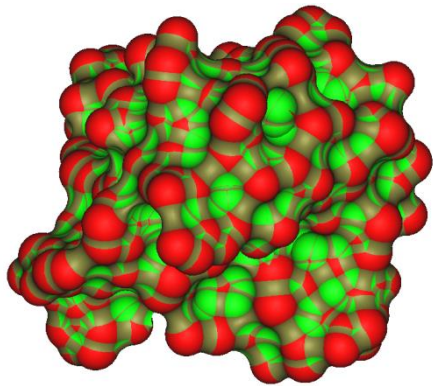


Molecular surface from RasMol (v2.7.3)



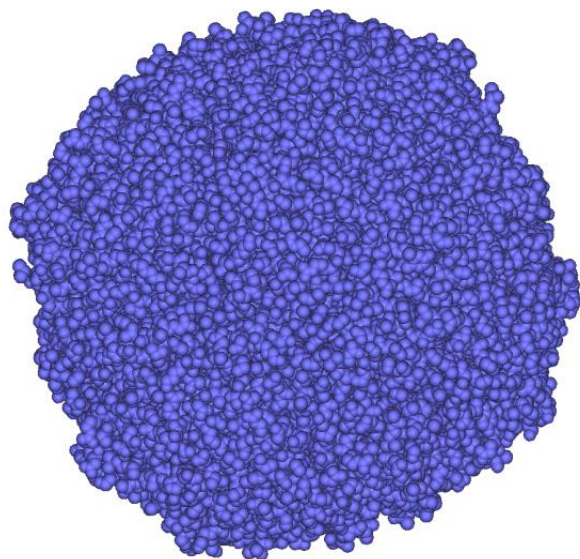
Molecular surface from BetaMol

Geometric Questions: Surfaces and Voids

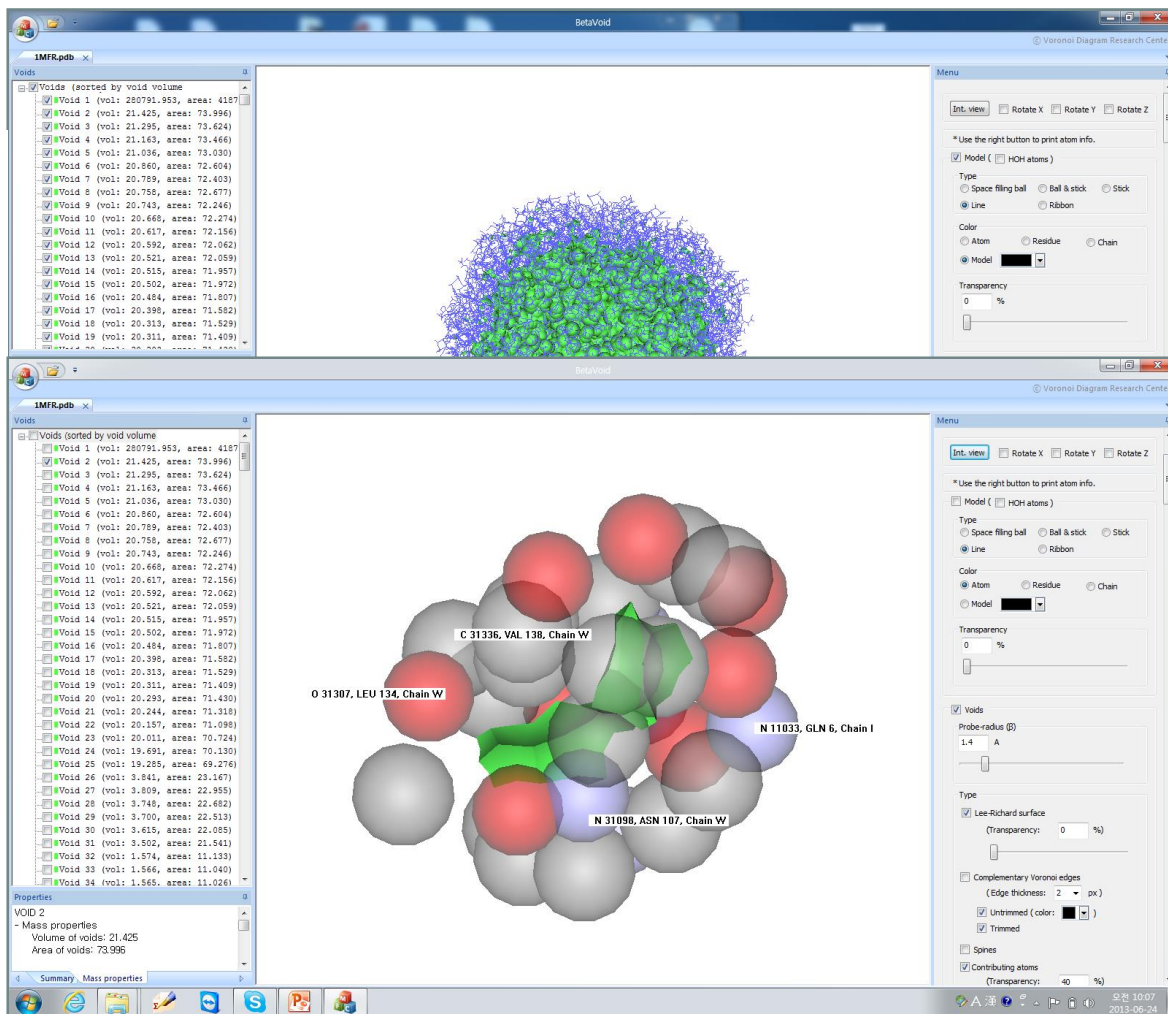


BetaVoid

(<http://voronoi.hanyang.ac.kr/software.htm>)



Ferritin
(1MFR, #atom: 32,952)



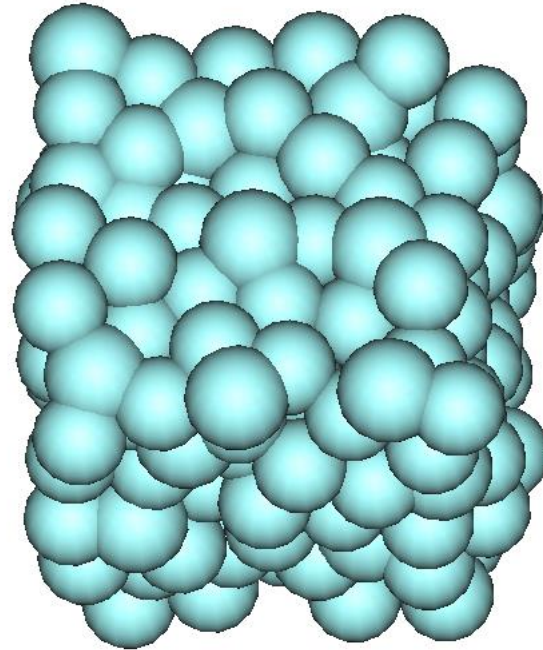
The software interface displays a list of voids sorted by volume, with the following data:

Void ID	Volume (vol)	Area
Void 1	280791.953	4187
Void 2	21.425	73.996
Void 3	21.295	73.624
Void 4	21.163	73.466
Void 5	21.036	73.030
Void 6	20.860	72.604
Void 7	20.789	72.403
Void 8	20.758	72.677
Void 9	20.745	72.246
Void 10	20.668	72.274
Void 11	20.617	72.156
Void 12	20.592	72.062
Void 13	20.521	72.059
Void 14	20.515	71.957
Void 15	20.500	71.973
Void 16	20.484	71.807
Void 17	20.398	71.582
Void 18	20.313	71.529
Void 19	20.311	71.409
Void 20	20.293	71.430
Void 21	20.244	71.310
Void 22	20.157	71.098
Void 23	20.011	70.724
Void 24	19.691	70.130
Void 25	19.285	69.276
Void 26	3.841	23.167
Void 27	3.809	22.955
Void 28	3.748	22.682
Void 29	3.700	22.513
Void 30	3.615	22.085
Void 31	3.502	21.543
Void 32	1.874	11.133
Void 33	1.566	11.040
Void 34	1.565	11.026

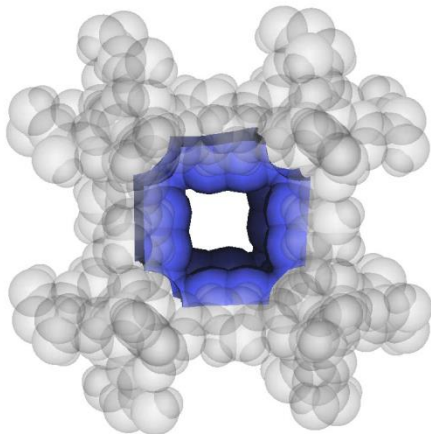
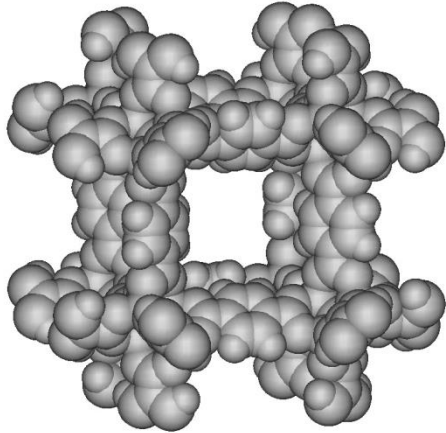
The bottom screenshot also shows the following labels for specific atoms:

- C 31336, VAL 138, Chain W
- O 31307, LEU 134, Chain W
- N 11033, GLN 6, Chain I
- N 31098, ASN 107, Chain W

Cavity in Amorphous Material



Metal Organic Framework (MOF)



■ Applications

- adsorption
- energy storage
- membrane, etc.

■ Critical Geometric Features

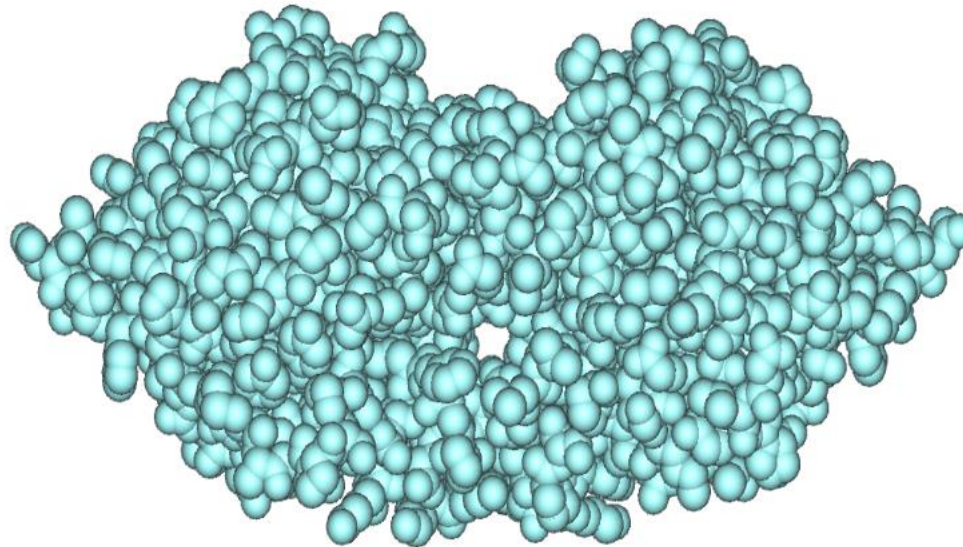
- Tunnel
- Pore (Void)

■ Other new materials

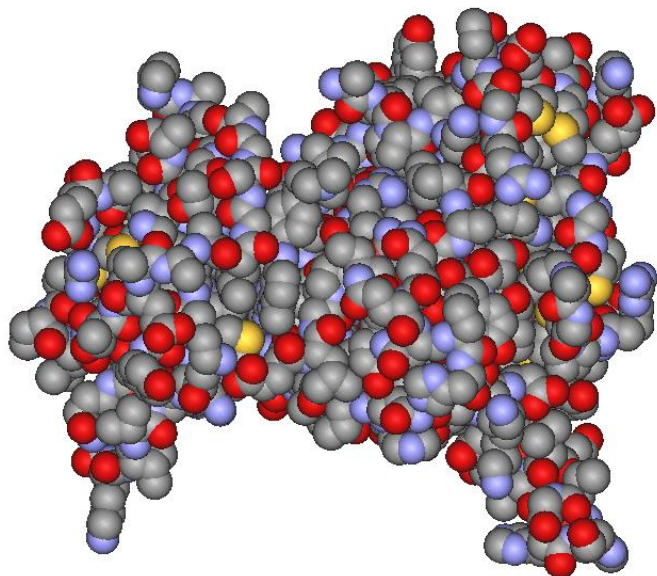
- Li-ion battery
- Membrane
- Fuel cell
- OLED
- Conducting polymer
- Etc.

Tunnels in proteins

- **Carbonic anhydrase XII (PDB ID: 1jd0 , #atom: 8142, #residue: 253)**



Volume and Boundary Area



Tyrosine Kinase(1XBA) + Gleevec

	Tyrosine Kinase(1XBA)
# of Atoms	2068

vdw Vol.(\AA^3)	22551.84
(time:sec)	0.016

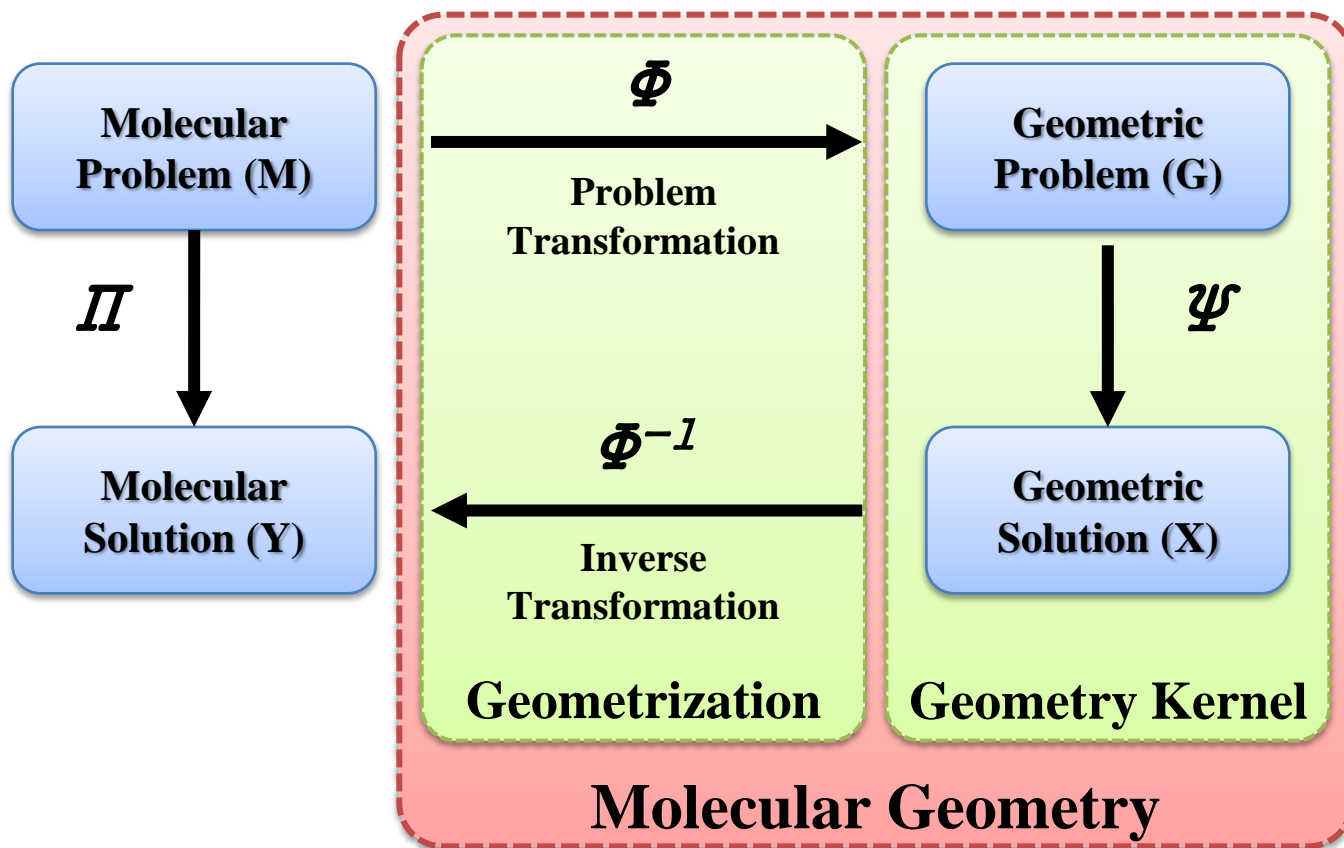
vdw Area(\AA^2)	26968.48
(time:sec)	0.031

VD (time:sec)	1.547
QT & BC (time:sec)	0.922

(Intel Core2 Duo, 3.0GHz, 3GB RAM)

MG / MGOS PARADIGM

Molecular Geometry: New Discipline



MGOS Application Program : an example

```
#include "MolecularGeometry.h"
using namespace MGOS;
```

→ Include header file

```
int main(int argc, char* argv[])
{
    string pdbFilename = argv[1];
```

```
MolecularGeometry MG;
MG.loadPDB( pdbFilename );
MG.preprocess();
```

→ Preprocess
(VD and QT)

```
// For van-der Waals model
```

```
cout << "# boundary atoms on van-der Waals model : "
      << MG.countNumberOfVDWalsBoundaryAtoms() << endl << endl;
```

```
MolecularMassProperty vdWMass = MG.computeVDWalsVolumeAndArea();
```

```
cout << "vdW volume    : " << vdWMass.getVolume() << endl;
cout << "vdW area      : " << vdWMass.getArea()  << endl << endl;
```

```
// For Lee-Richards model
```

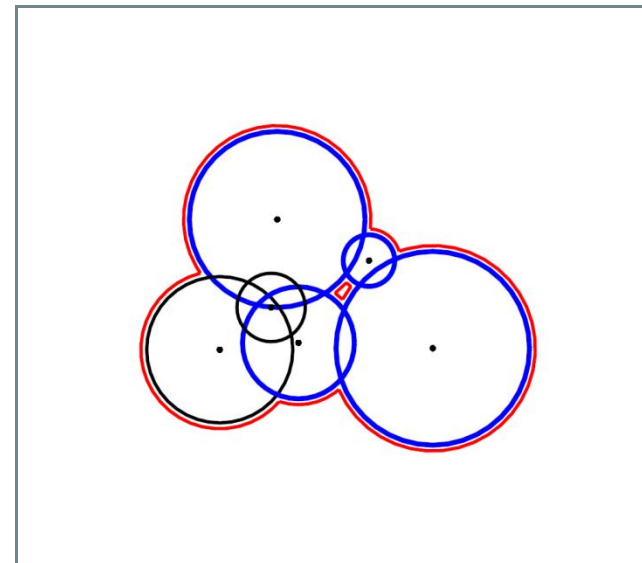
```
double water = 1.4;
cout << "# boundary atoms on LR model: "
      << MG.countNumberOfLeeRichardsBoundaryAtoms(water) << endl << endl;
```

```
MolecularMassProperty LRMass = MG.computeLeeRichardsVolumeAndArea(water);
cout << "LR volume    : " << LRMass.getVolume() << endl;
cout << "LR area      : " << LRMass.getArea()  << endl << endl;
```

```
MolecularVoidSet LRVoids = MG.computeLeeRichardsVoids( water );
cout << "# voids      : " << LRVoids.countNumberOfVoids() << endl;
```

```
MolecularVoid largestVoid = LRVoids.getLargestVoid();
cout << " Volume of largest void    : " << largestVoid.getVolume() << endl;
cout << " Boundary area of largest void : " << largestVoid.getArea() << endl;
```

```
AtomArrangement atoms = largestVoid.getContributingAtoms();
for ( AtomIterator i_atom=atoms.begin(); i_atom!=atoms.end(); i_atom++, i++ ) {
    cout << " atom " << i << " : ";
    cout.precision(3);
    cout << largestVoid.getAreaContributedByAtom( *i_atom ) << endl;
}
```



Count boundary atoms of VDW model

Compute
volume and area of VDW model

Count boundary atoms of LR model

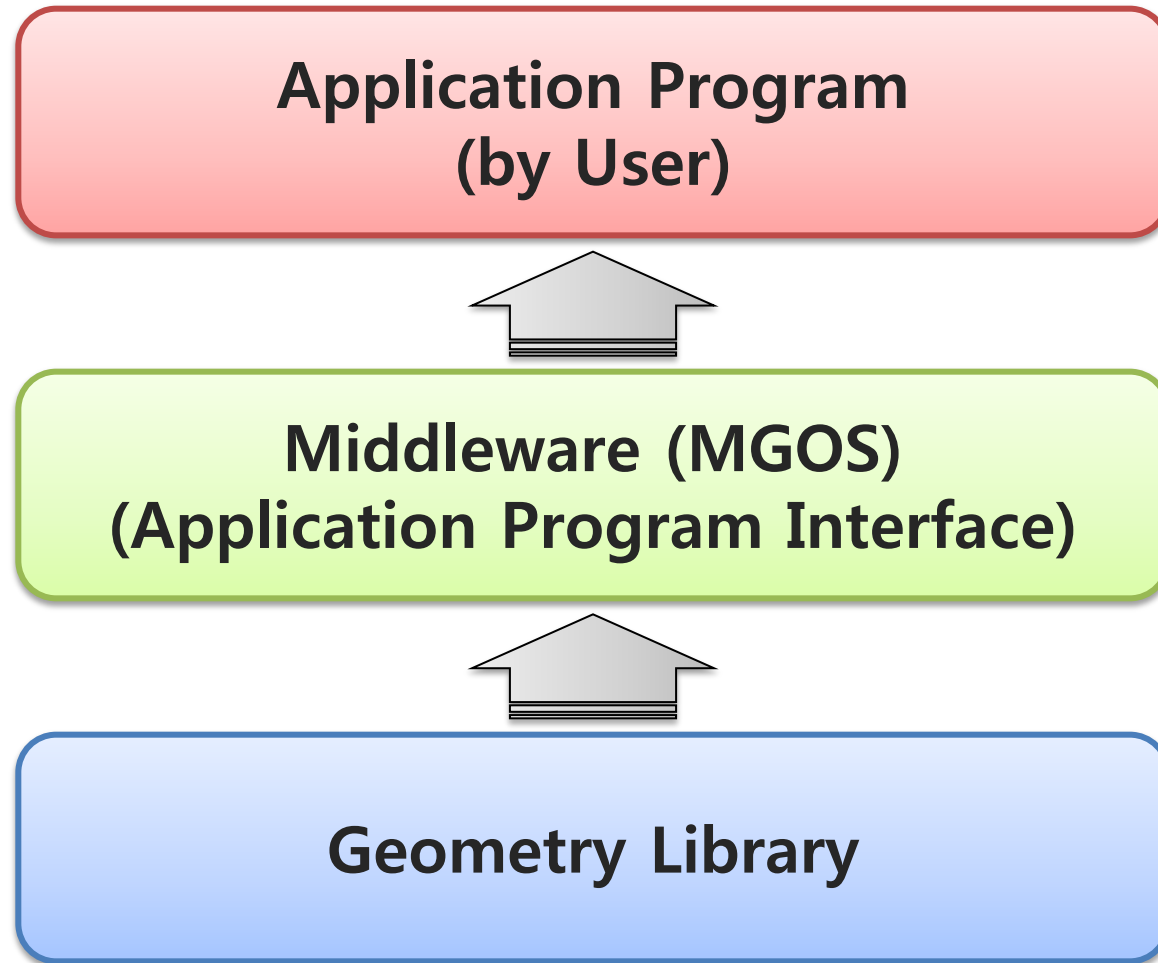
Compute
volume and area of LR model

Compute and count
LR voids

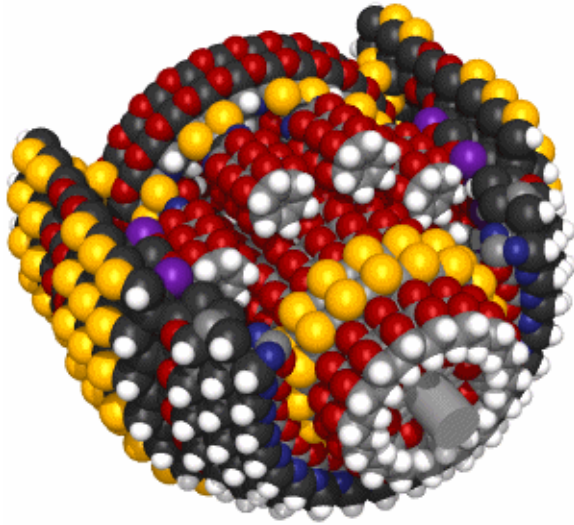
Volume/area
of largest LR void

Contributing area for each atom
of largest LR void

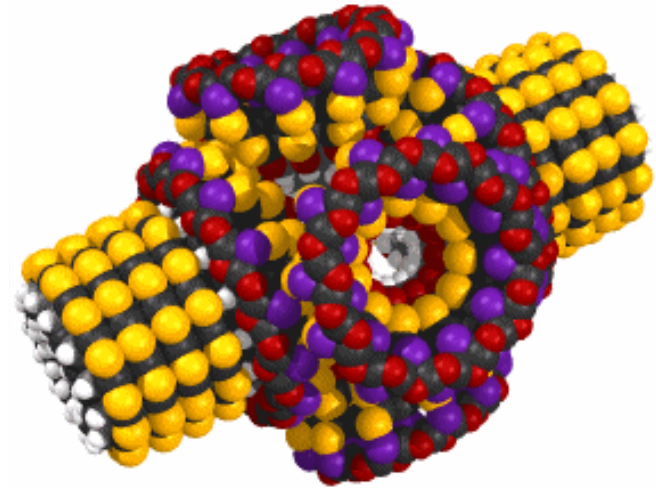
MGOS Architecture



Nano Machinery Design



MarkIII(k) Planetary Gear



Drexler-Merkle Differential Gear

Designed by K. Drexler (<http://www.nanorex.com>)

MG/MM/MD/QM

**Core Building Block
For MGI**

Designing molecules with new functions...

(Precompetitive 20 projects...)

Theory, modeling & simulation: x1000 faster...

(12 Global trends to 2020)

From Mihail Roco, Sep 29, 2014

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- Prof. Andreas Dress (Bielefeld U, Germany)

- Dr. Jong Bhak (Teragen Inc.)
- Prof. Seung Eon Ryu (Life Engineering Dept., Hanyang U)
- Dr. Roman Laskowski (European Bioinfo Inst, UK)
- Prof. Chaok Seok (Chemistry, SNU)
- many others....



Thank You

<http://voronoi.hanyang.ac.kr>