

# LEGO® Molecular-Scale Models

## *Building Instructions for Structures at the Molecular Scale*

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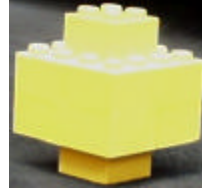
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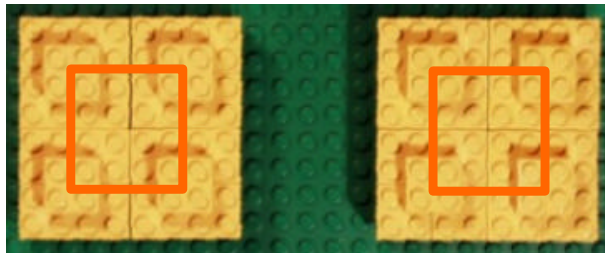
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# Simple Cubic

LEGO unit  
representing atoms  
in this structure:

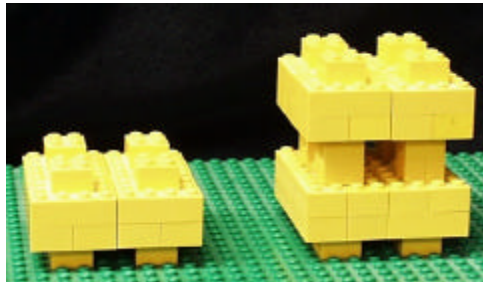


Whole atoms:

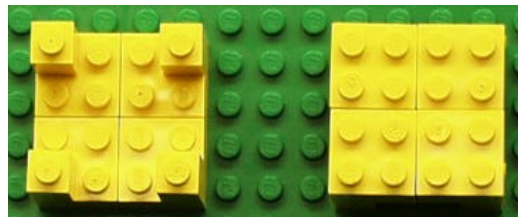


**Z=0**

**Z=1**

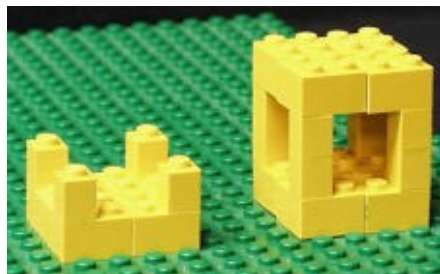


Unit cell:



**Z=0**

**Z=1**





# Body-Centered Cubic (whole atoms)

LEGO unit representing  
atoms in this structure:



This atom model requires:

4 yellow 2x4 bricks

2 yellow 2x2 bricks

NOTE: The red LEGOs depict portions of the  
structure within the unit cell.

This model requires:

24 yellow 2x4 bricks

8 yellow 2x2 bricks

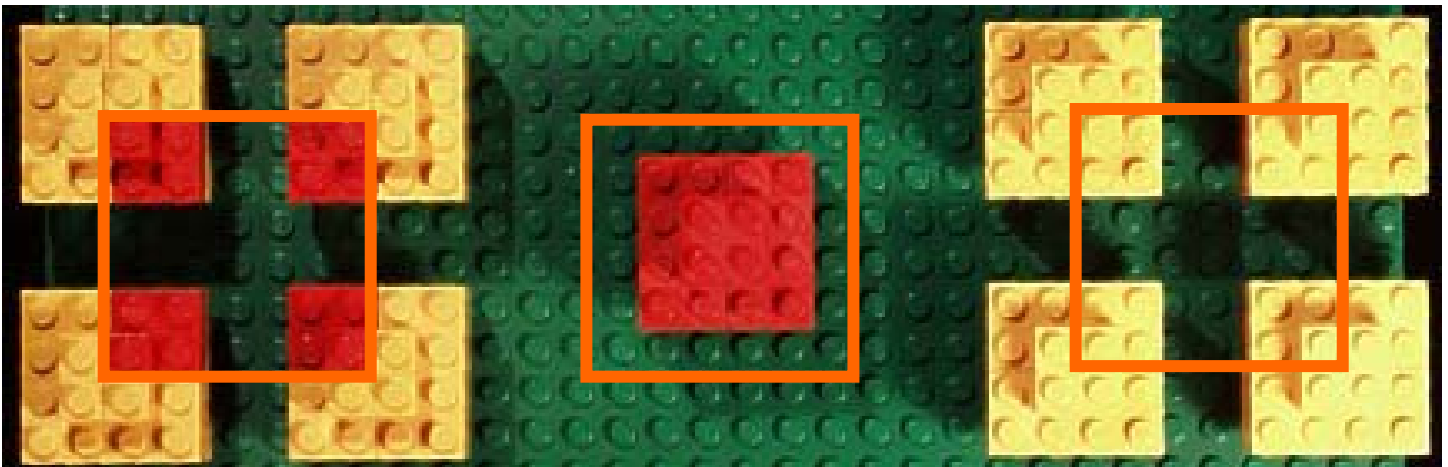
8 yellow 1x2 bricks

8 yellow 1x1 bricks

4 red 2x4 bricks

6 red 2x2 bricks

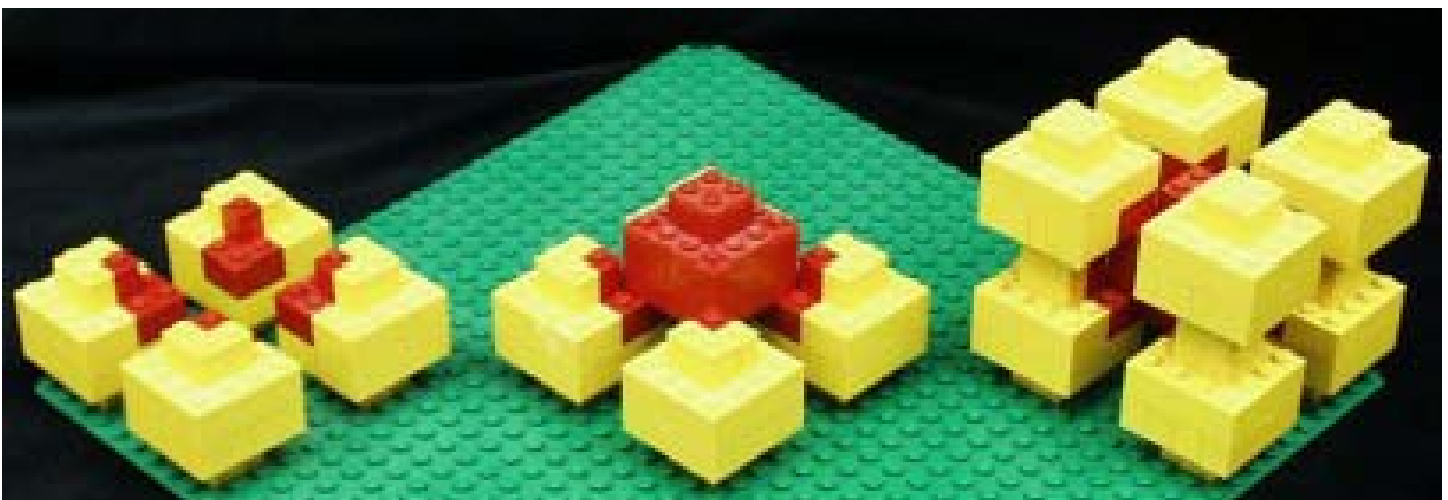
8 red 1x1 bricks



**Z=0**

**Z=1/2**

**Z=1**



# Face Centered Cubic (whole atoms)

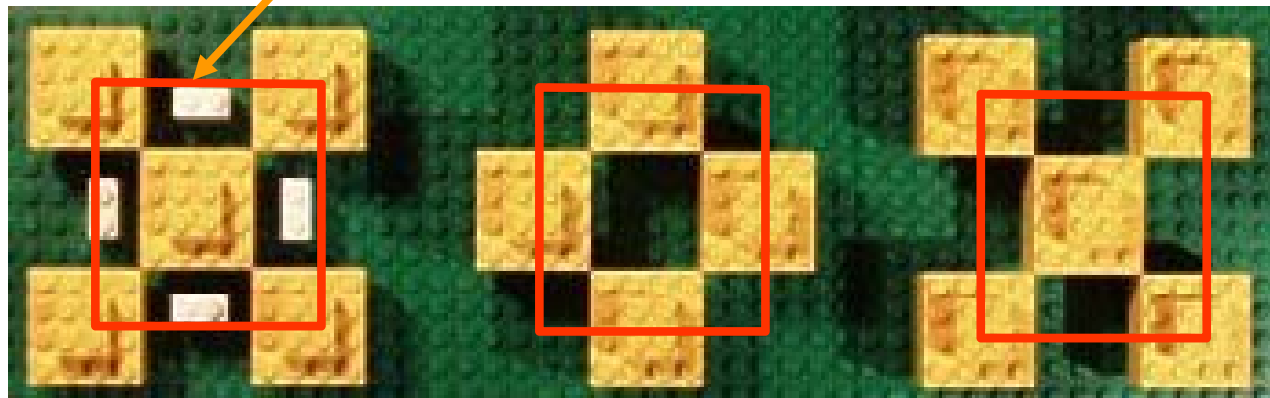
LEGO unit representing  
atoms in this structure:



This atom model requires:  
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:  
56 yellow 2x4 bricks  
28 yellow 2x2 bricks  
8 black 1x2 bricks

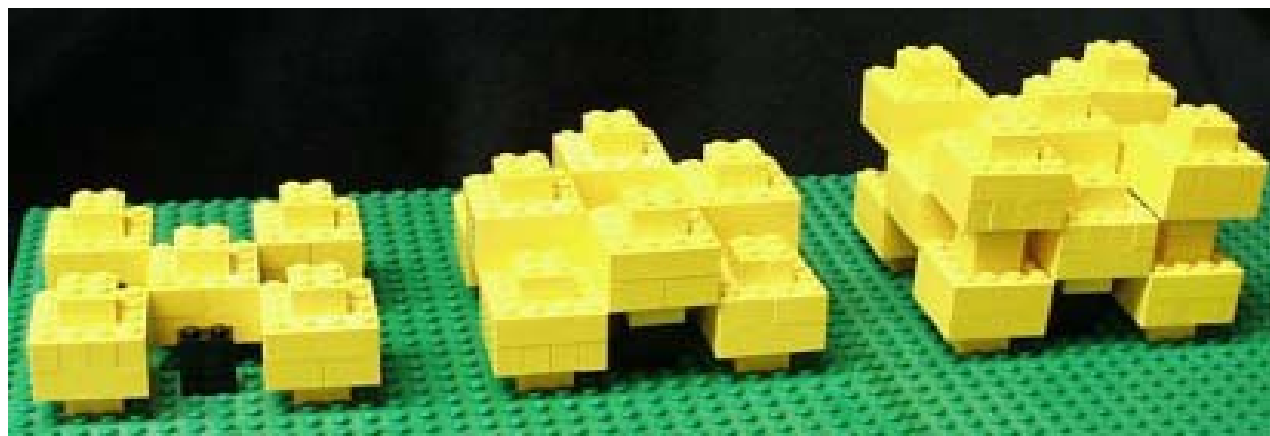
These are supports made  
from two 1x2 bricks.



**Z=0**

**Z=1/2**

**Z=1**



# Face Centered Cubic (unit cell)

LEGO unit representing  
atoms in this structure:



This atom model requires:

4 yellow 2x4 bricks

2 yellow 2x2 bricks

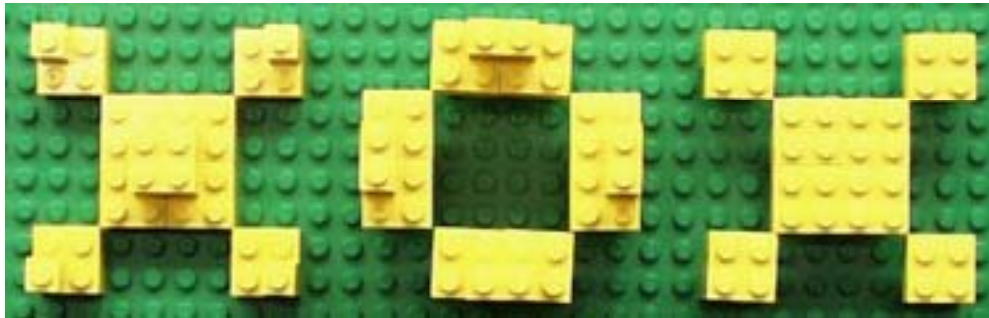
This model requires:

14 yellow 2x4 bricks

9 yellow 2x2 bricks

8 yellow 1x2 bricks

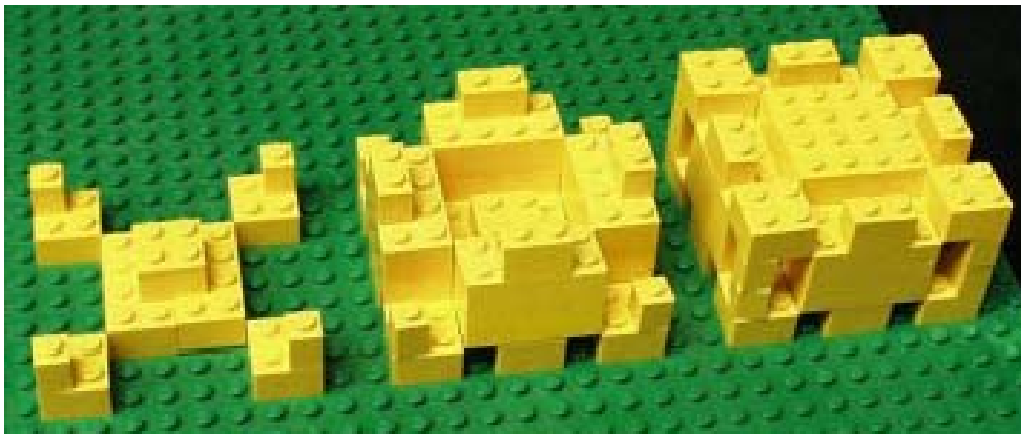
8 yellow 1x1 bricks



**Z=0**

**Z=1/2**

**Z=1**



# Hexagonal Close-Packing Layers (whole atoms)

LEGO unit representing atoms in this structure:

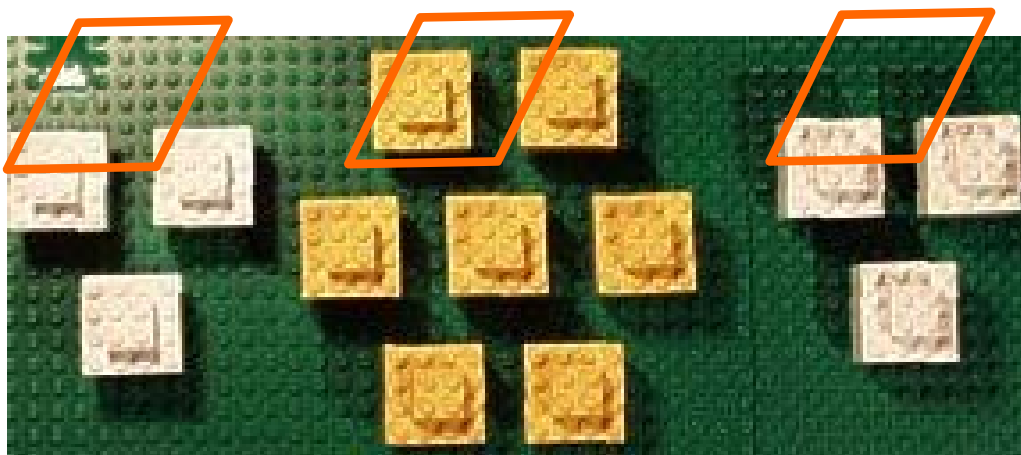


This atom model requires:  
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:

28 yellow 2x4 bricks	24 white 2x4 bricks
14 yellow 2x2 bricks	12 white 2x2 bricks

Note: Colors distinguish layers.



**Z=0**

**Z=1/2**

**Z=1**



# Cubic Close Packing Layers (whole atoms)

LEGO unit representing  
atoms in this structure:



This atom model requires:

4 yellow 2x4 bricks

2 yellow 2x2 bricks

Note: Colors distinguish layers.

Layer A is white,  
layer B is yellow,  
and layer C is red.

This model requires:

28 yellow 2x4 bricks

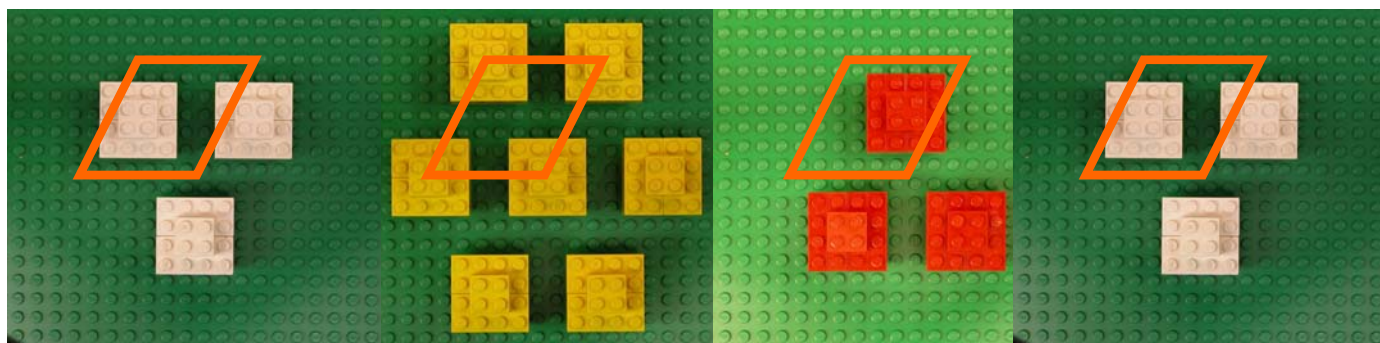
14 yellow 2x2 bricks

24 white 2x4 bricks

12 white 2x2 bricks

12 red 2x4 bricks

6 red 2x2 bricks

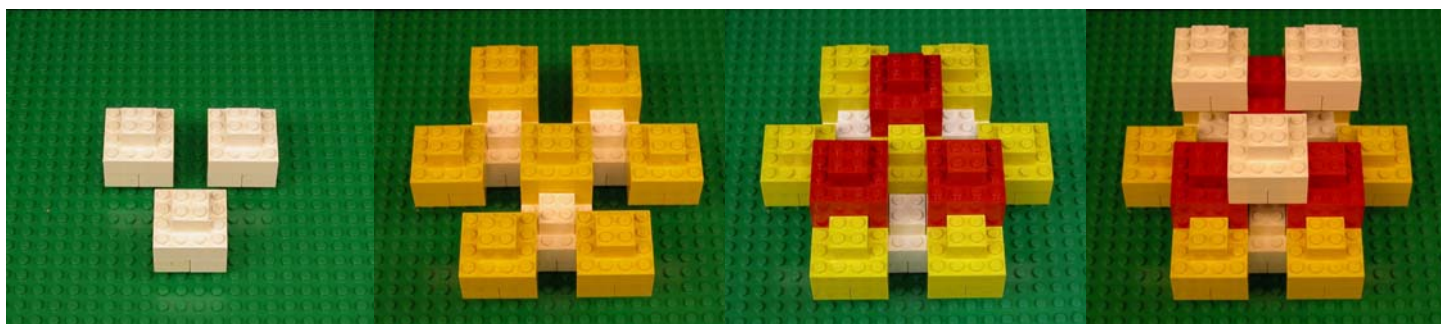


**Z=0**

**Z=0.333**

**Z=0.667**

**Z=1**





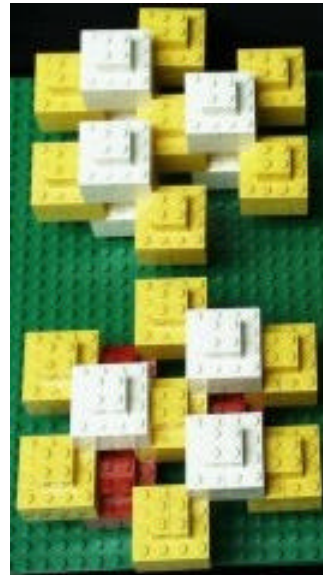
# Close-Packed Structures

LEGO unit representing atoms in this structure:



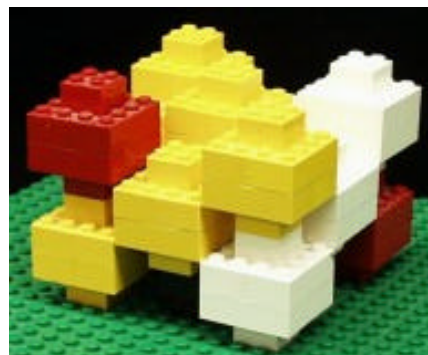
Note: Colors distinguish layers.  
Layer A is white, layer B is yellow, and layer C is red.

Hexagonal  
close-packed  
(ABAB... layers)



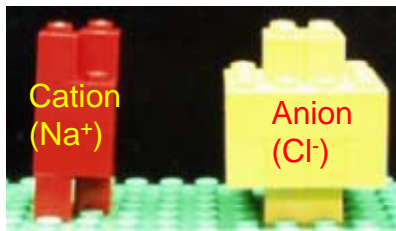
Cubic  
close-packed  
(ABCABC... layers)

Note: The cubic close-packed structure is the **same** as the face-centered cubic structure. The layers are simply oriented differently.



# Rock Salt (whole ions)

LEGO units  
representing  
different-sized ions  
in this structure:

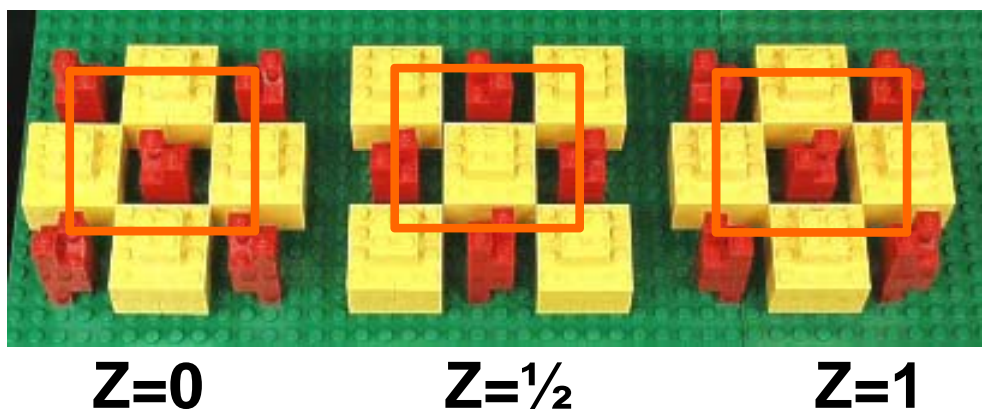


This atom model requires:

4 yellow 2x4 bricks  
2 yellow 2x2 bricks  
2 red 2x2 bricks  
4 red 1x1 bricks

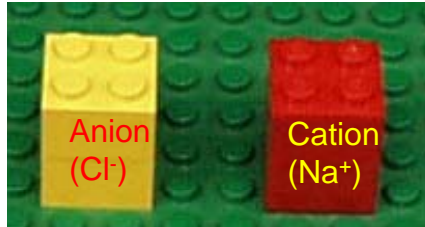
This model requires:

52 yellow 2x4 bricks    28 red 2x2 bricks  
26 yellow 2x2 bricks    56 red 1x1 bricks



# Rock Salt (unit cell)

LEGO units  
representing ions  
in this structure:



This atom model requires:  
2 red 2x2 bricks  
2 yellow 2x2 bricks

This model requires:

1 yellow 2x2 brick    2 red 2x2 bricks  
8 yellow 1x2 bricks    4 red 1x2 bricks  
4 yellow 1x1 bricks    5 red 1x1 bricks



**Z=0**

**Z=1/2**

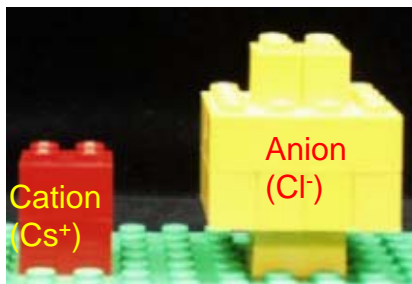
**Z=1**





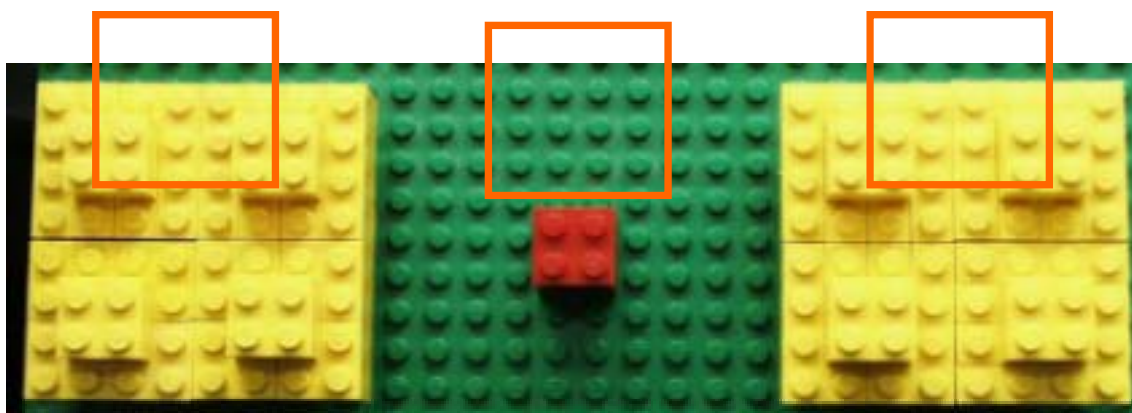
# Cesium Chloride (whole ions)

LEGO units representing  
ions in this structure:



This atom model requires:  
4 yellow 2x4 bricks  
2 yellow 2x2 bricks  
2 red 2x2 bricks

This model requires:  
32 yellow 2x4 bricks  
16 yellow 2x2 bricks  
2 red 2x2 bricks



**Z=0**

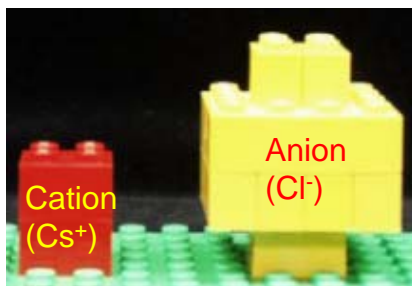
**Z=1/2**

**Z=0**



# Cesium Chloride (unit cell)

LEGO units representing  
ions in this structure:



This atom model requires:

4 yellow 2x4 bricks  
2 yellow 2x2 bricks  
4 red 1x2 bricks

This model requires:

8 yellow 2x4 bricks  
8 yellow 1x1 bricks  
4 red 1x2 bricks



**Z=0**

**Z=1/2**

**Z=1**



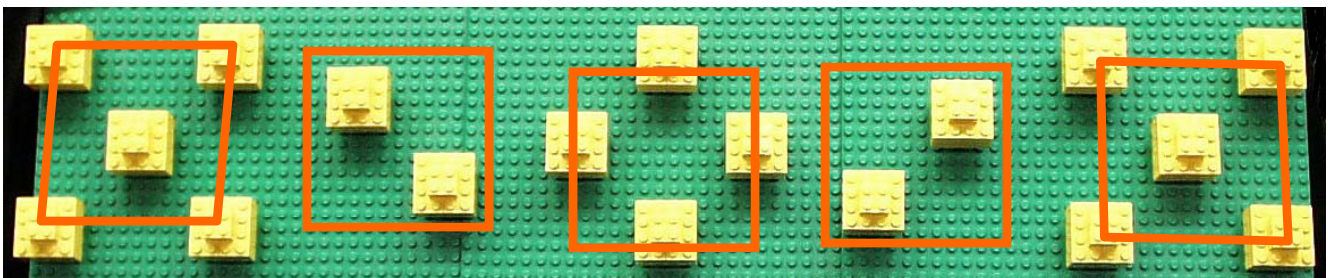
# Diamond (whole atoms)

LEGO unit representing  
atoms in this structure:



This atom model requires:  
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:  
72 yellow 2x4 bricks  
36 yellow 2x2 bricks  
16 black 1x1 bricks



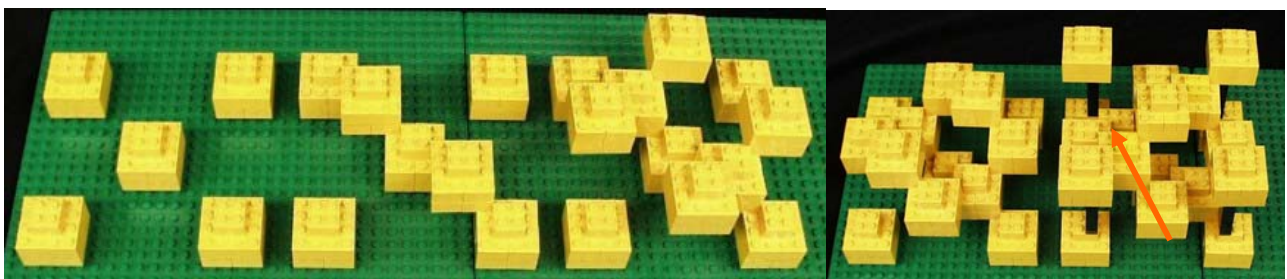
**Z=0**

**Z=1/4**

**Z=1/2**

**Z=3/4**

**Z=1**



These are supports  
made from four 1x1  
bricks.

Side view  
of diamond  
structure:



Tetrahedral bonding  
in diamond structure:





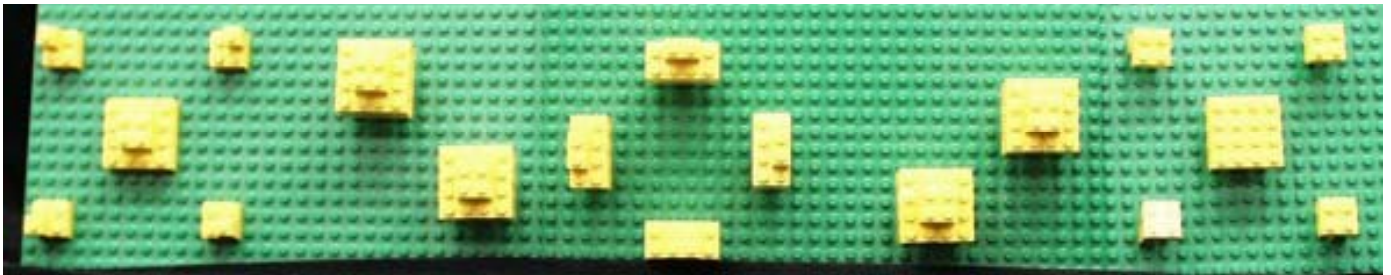
# Diamond Unit Cell

LEGO unit representing atoms in this structure:



This atom model requires:  
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:  
28 yellow 2x4 bricks  
18 yellow 2x2 bricks  
4 yellow 1x2 bricks  
8 yellow 1x1 bricks  
8 black 1x2 bricks



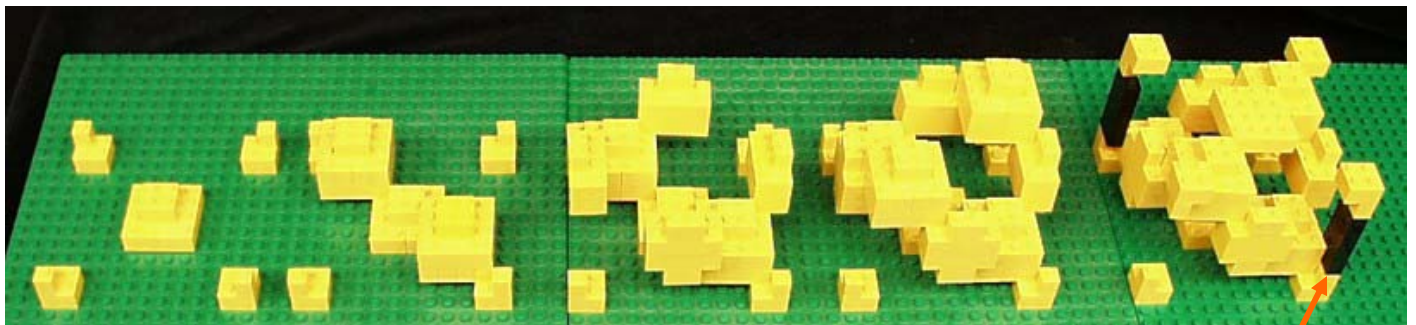
**Z=0**

**Z=1/4**

**Z=1/2**

**Z=3/4**

**Z=1**



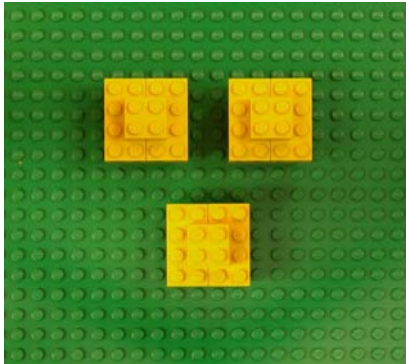
These are supports  
made from four 1x2  
bricks.

# Diamond vs. Lonsdaleite (whole atoms)

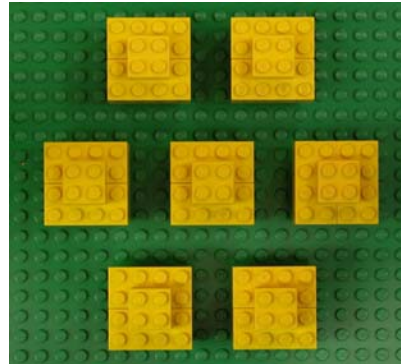
LEGO unit representing atoms in this structure:



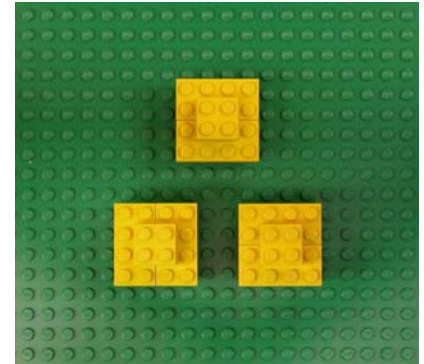
The carbon atoms in both structures are bonded to the other carbon atoms in a tetrahedral geometry:



**“A” Layer**

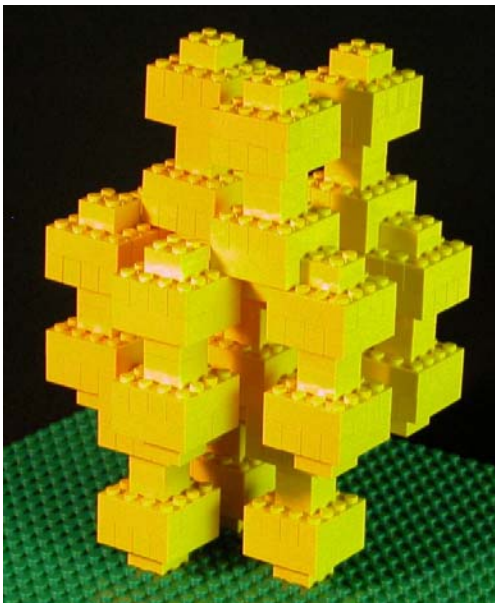


**“B” Layer**

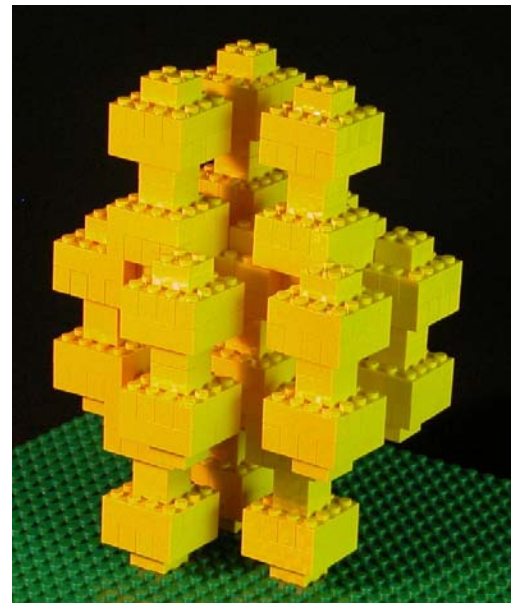


**“C” Layer**

Angle view of diamond structure  
(Layers **AABBCCBBAABBCCBB...**):



Angle view of lonsdaleite structure  
(Layers **AABBAABBAABBA...**):



# Graphite (whole atoms)

LEGO unit representing  
atoms in this structure:



Note: The spacers (10 pegs long) should be perpendicular to each layer of graphite to show the scale of spacing between the layers.

This layer requires:  
64 yellow 2x4 bricks  
32 yellow 2x2 bricks





# $C_{60}$ and $C_{70}$ Buckminsterfullerenes (whole atoms)

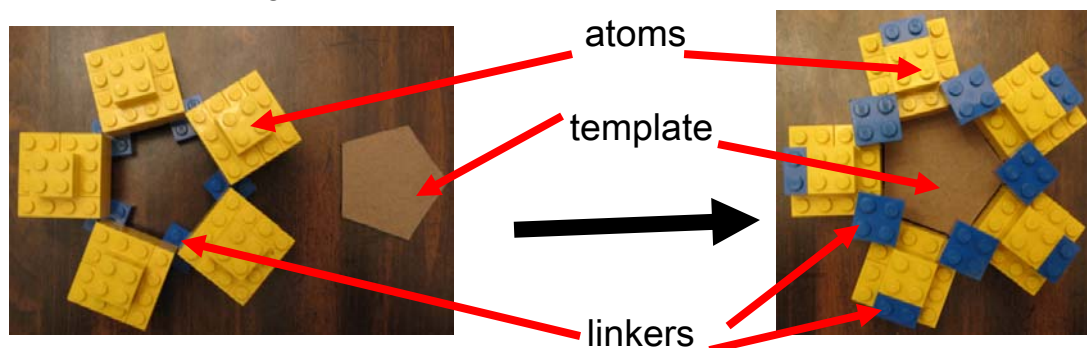
These are the most challenging (and rewarding) builds that I have attempted, and the resulting models have the same atom connectivity as  $C_{60}$  and  $C_{70}$  molecules. I recommend using fresh bricks with snug tolerances, a careful eye for symmetry, and a good dose of patience. This structure uses both support posts (which one might be able to carefully remove after the fullerene structure is complete and maybe even glued) and small bricks (2x2 and 1x2) to link the atoms together. Enjoy! -DJC-

LEGO unit representing  
atoms in this structure:



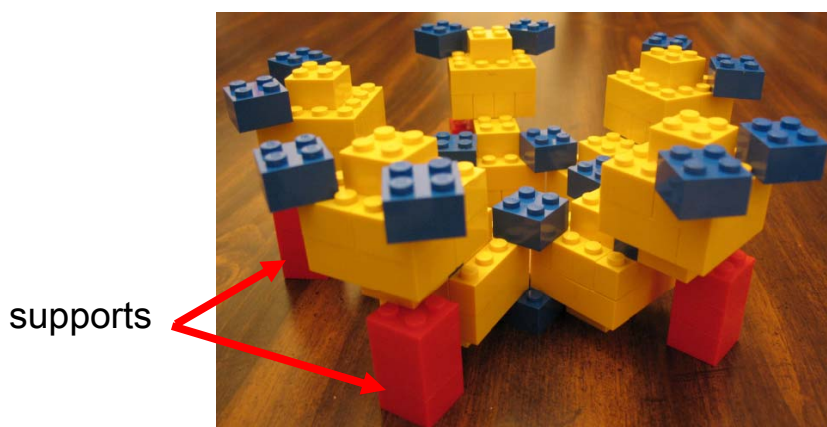
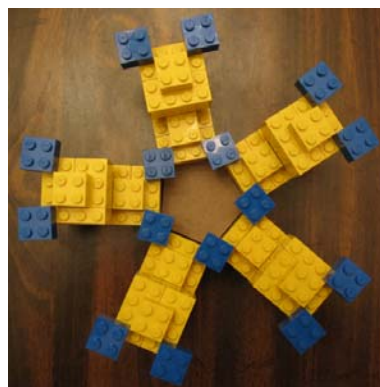
Level 1: 5 atoms, 10 2x2 linkers, 5 1x2 linkers

NOTE: Since this is the foundation level, it is helpful to build as perfect of a pentagon of the five atoms as possible. To accomplish this, made a cardboard pentagon template with about 31 mm edges to fit inside the ring of bricks.



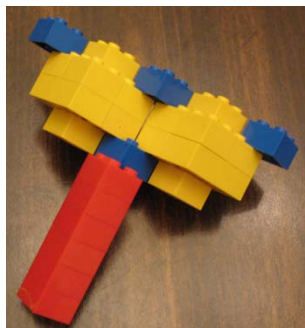
Level 2 added: 5 atoms, 10 2x2 linkers, 5 supports (3 bricks high)

NOTE: Using 2x2 bricks for the supports, and connecting them to the atoms by only one peg, is a trade off between model stability and ease of support removal later on.

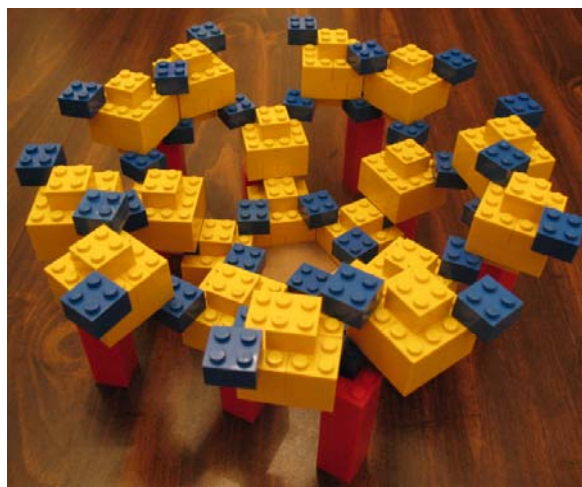
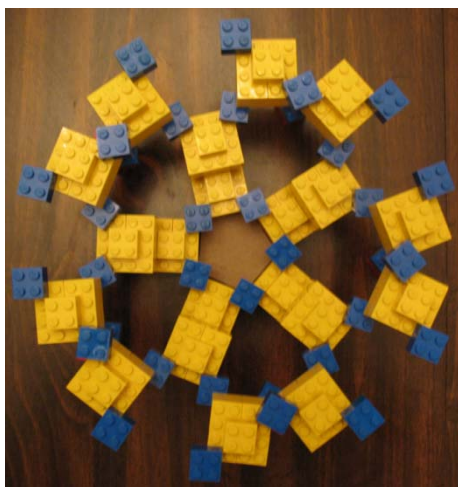


Level 3 added: 10 atoms, 20 2x2 linkers, 5 supports (6 bricks high)

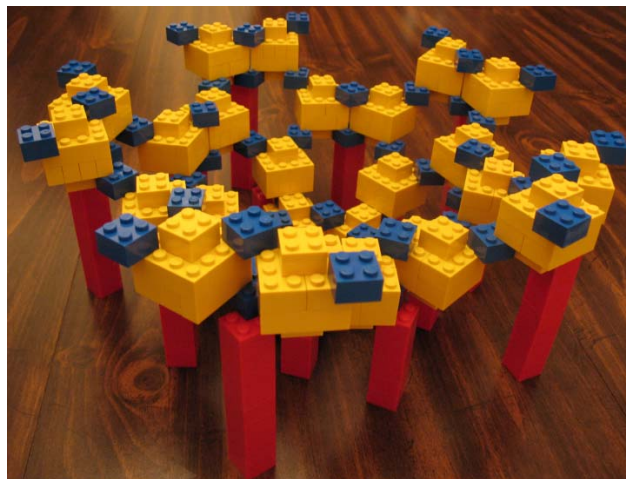
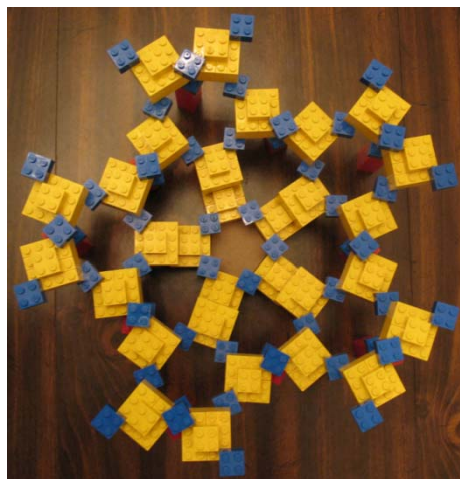
NOTE: The 2x2 linkers must be turned to connect the atoms together. It helps to add atoms in linked pairs.



Linked pair  
and support



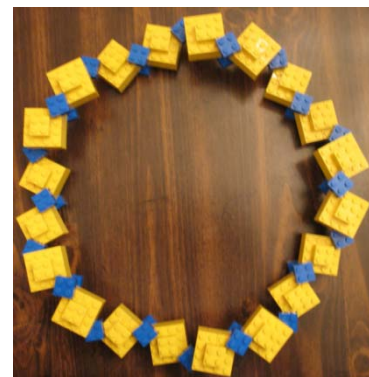
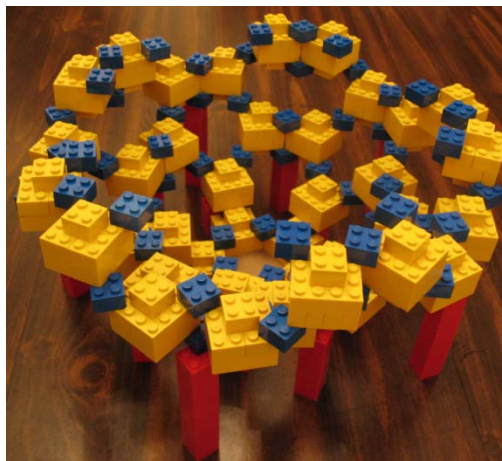
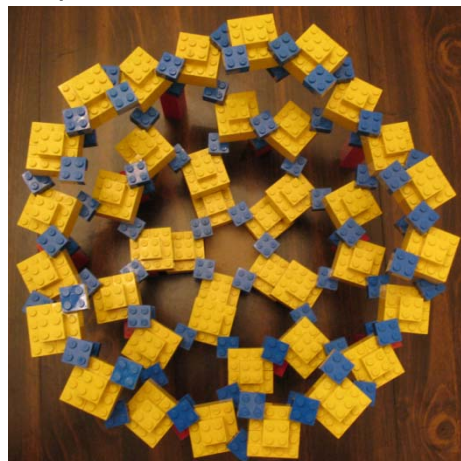
Level 4 added: 10 atoms, 20 2x2 linkers, 5 supports (9 bricks high)



Level 5 added: 10 atoms, 20 2x2 linkers

NOTE: The pattern of atoms in Level 5 is similar to that of Level 4, only rotated by 36°.

Levels 4 and 5 contain the “equator” of the structure and should make as uniform of a ring together as possible.



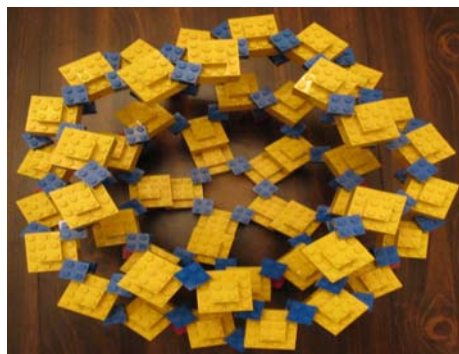
Levels 4 and 5  
together make a ring

Modifications to make  $C_{70}$  are described on the last page.



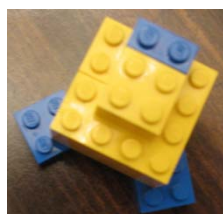
## Level 6 added: 10 atoms, 10 2x2 linkers

NOTE: The pattern of atoms in Level 6 is similar to that of Level 3, only rotated by  $36^\circ$ .

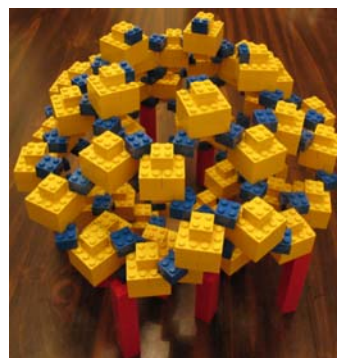


## Level 7 added: 5 atoms, 10 2x2 linkers, 5 1x2 linkers

NOTE: It helps to add atoms as the units shown. The pattern of atoms in Level 7 is similar to that of Level 2, only rotated by  $36^\circ$ .

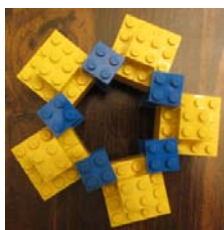
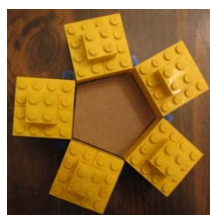


One atom  
and 3 linkers

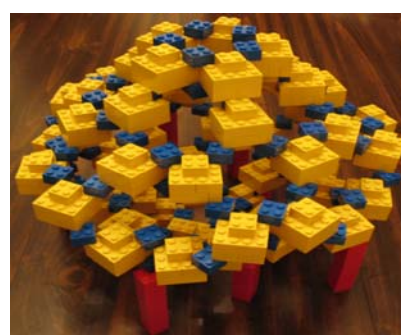


## Level 8 added: 5 atoms, 10 2x2 linkers

NOTE: It helps to add this level by building a 5-atom ring and then adding the entire level at once. The level should just be able to rest in place, but fastening this level down to Level 7 makes for a stronger and better-looking structure. The pattern of atoms in Level 8 is similar to that of Level 1, only rotated by  $36^\circ$ .



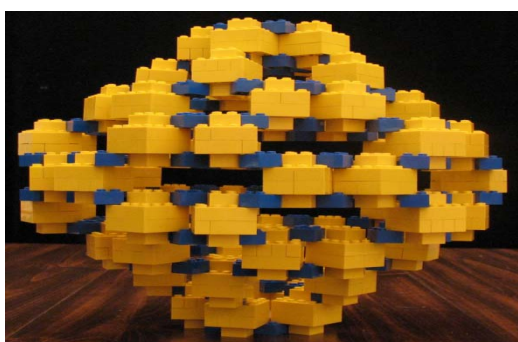
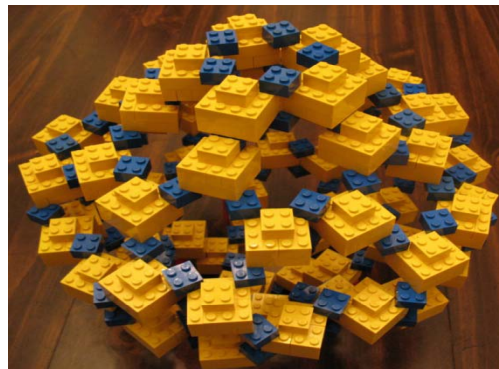
A template  
can help  
build the  
pentagon



This model ( $C_{60}$ ) requires:

- 240 yellow 2x4 bricks
- 120 yellow 2x2 bricks
- 90 red 2x2 bricks
- 110 blue 2x2 bricks
- 10 blue 1x2 bricks

To make  $C_{70}$ , add a Level “5 and a half”: 10 atoms, 20 2x2 linkers  
 This level would look like Level 4. If this extra level is used, Levels 6, 7, and 8 would not be rotated by  $36^\circ$  from Levels 3, 2, and 1.



Remember that these structures are fragile.



This model ( $C_{70}$ ) requires:

280 yellow 2x4 bricks

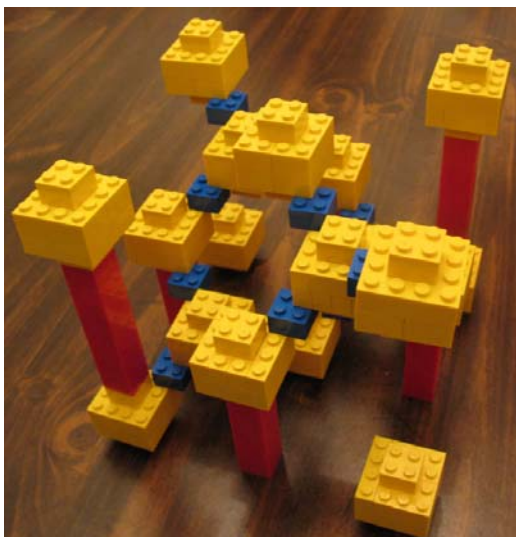
130 blue 2x2 bricks

140 yellow 2x2 bricks

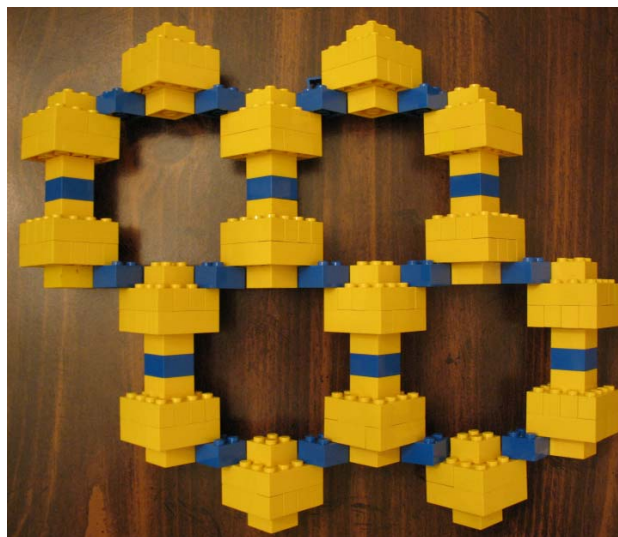
10 blue 1x2 bricks

90 red 2x2 bricks

Diamond and graphite models with linking bricks between the atoms can also be made for comparison to the fullerenes.



Diamond



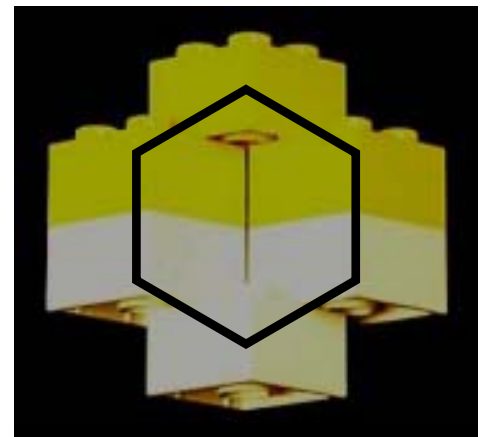
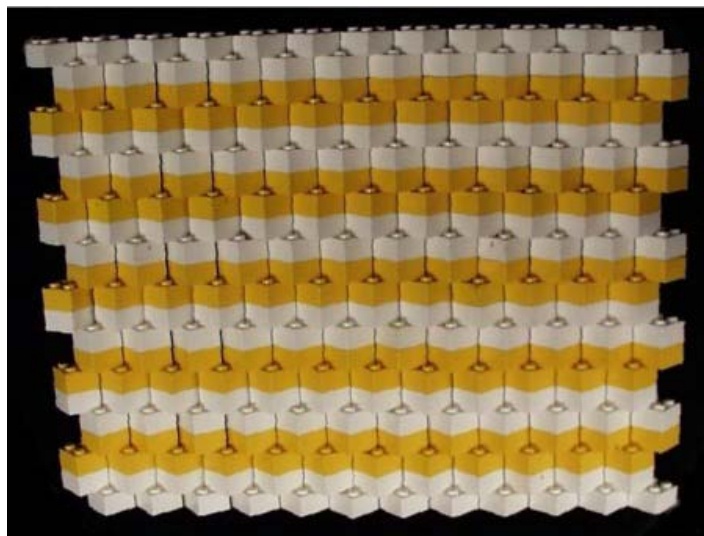
Graphite



# Buckytubes (whole atoms)

Carbon nanotubes, also known as buckytubes, can be thought of as a rolled-up graphite sheet. A simple representation of a flat graphite sheet is shown below. (For more sophisticated models of graphite, see the graphite building instructions.)

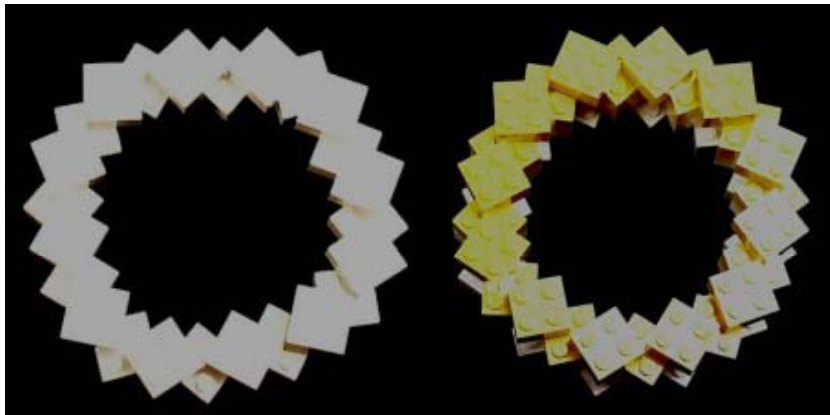
To build a simple graphite structure, build corner-connected chains of 2x2 bricks. Then stack several chains as shown.



These six 2 peg x 2 peg bricks represent a hexagon of carbon atoms, a fundamental part of graphite and buckytube structure. The different colors are used simply to distinguish individual bricks (atoms).

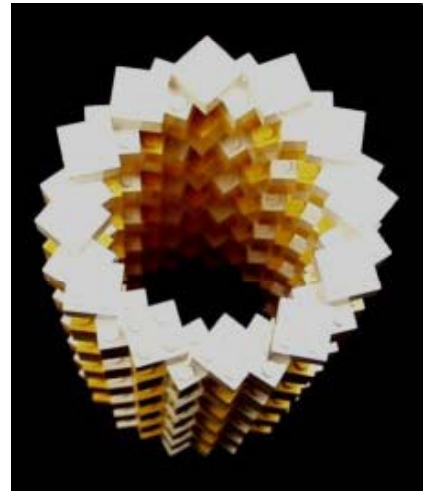
This model requires:  
Approximately 264  
2x2 bricks

Building the graphite structure above into a tube makes a portion of a buckytube structure.

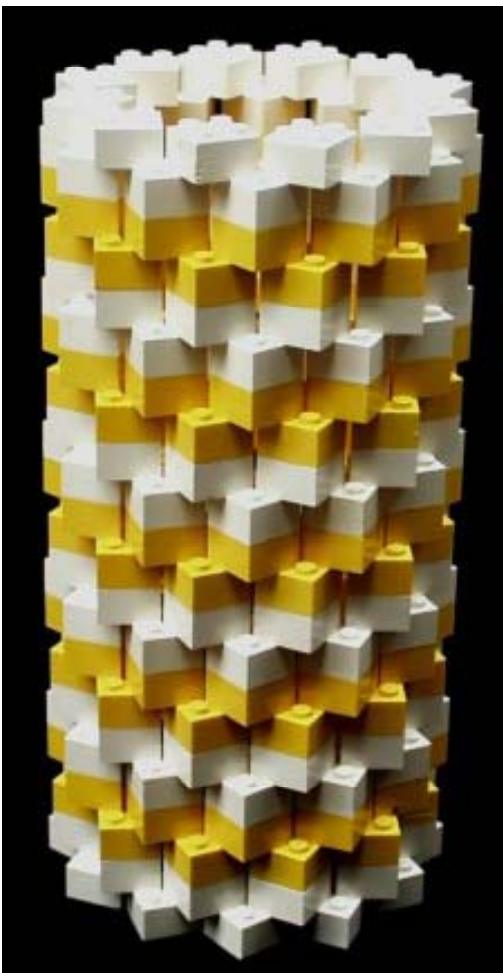


One chain

Two chains

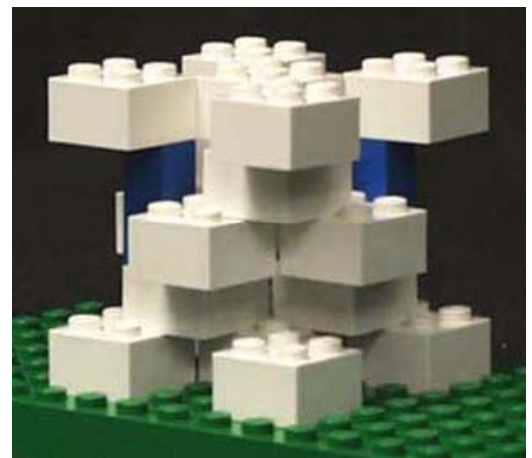


Eleven chains



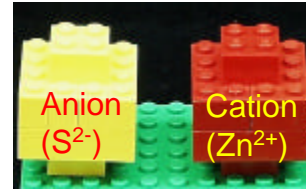
If each brick represents a carbon atom, then in real life this tube would be about a nanometer in diameter.

Note how different the graphite and buckytube structures are from the diamond structure. (For more sophisticated models of diamond, see the diamond building instructions.)

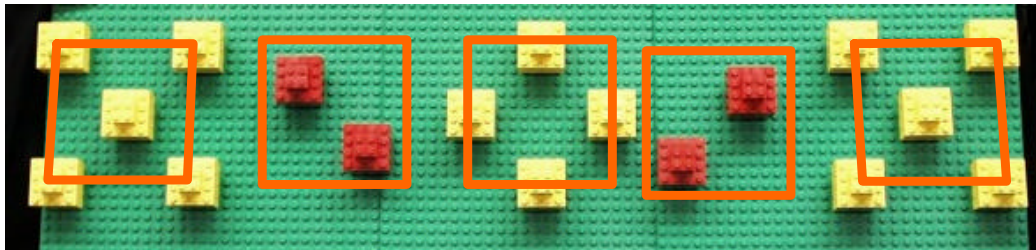


# Zinc Blende

LEGO unit representing  
ions in this structure:



Whole  
ions:



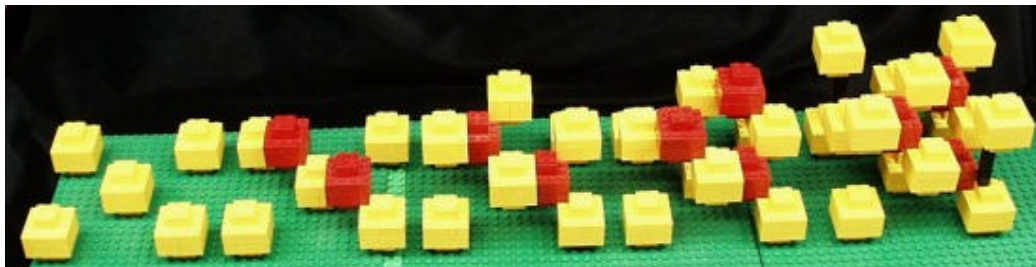
**Z=0**

**Z=1/4**

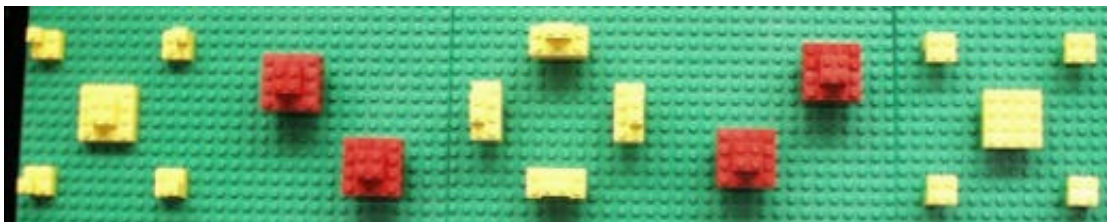
**Z=1/2**

**Z=3/4**

**Z=1**



Unit  
cell:



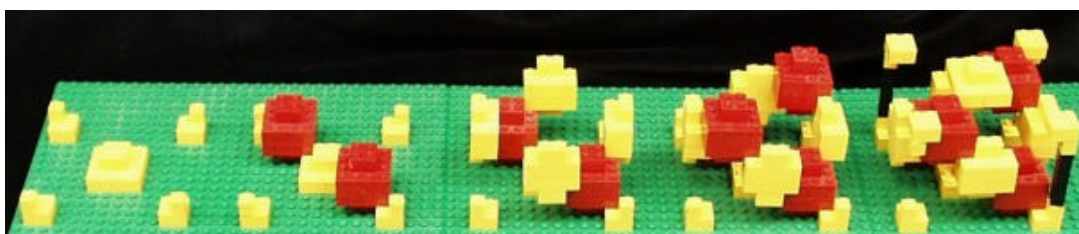
**Z=0**

**Z=1/4**

**Z=1/2**

**Z=3/4**

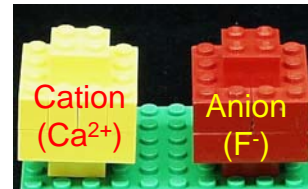
**Z=1**



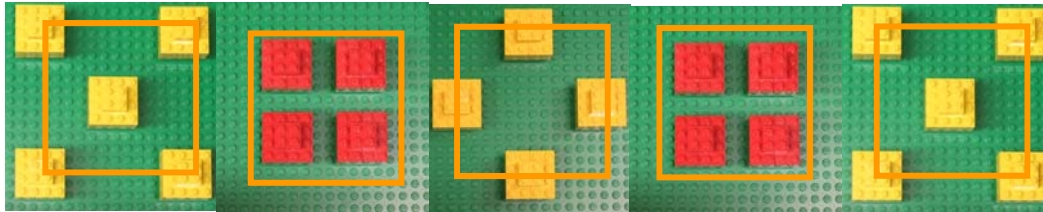


# Fluorite

LEGO unit representing  
ions in this structure:



Whole  
ions:



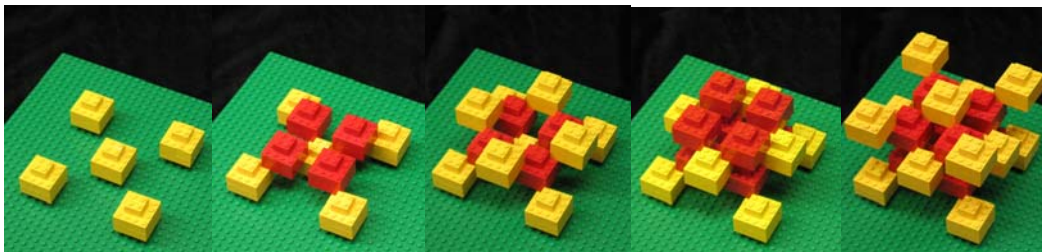
**Z=0**

**Z=1/4**

**Z=1/2**

**Z=3/4**

**Z=1**



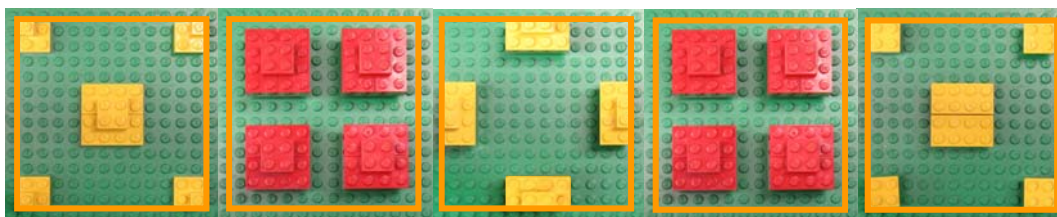
This model Whole ion requires:

56 yellow 2x4 bricks  
28 yellow 2x2 bricks  
32 red 2x4 bricks  
16 red 2x2 bricks

This model Unit cell requires:

12 yellow 2x4 bricks    32 red 2x4 bricks  
10 yellow 2x2 bricks    16 red 2x2 bricks  
8 yellow 1x2 bricks  
8 yellow 1x1 bricks

Unit  
cell:



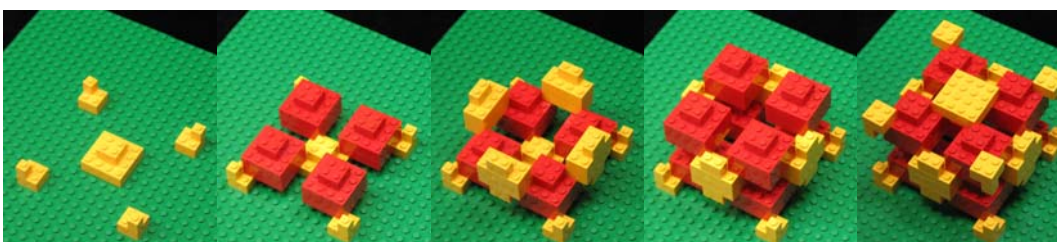
**Z=0**

**Z=1/4**

**Z=1/2**

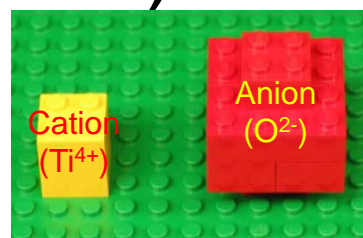
**Z=3/4**

**Z=1**

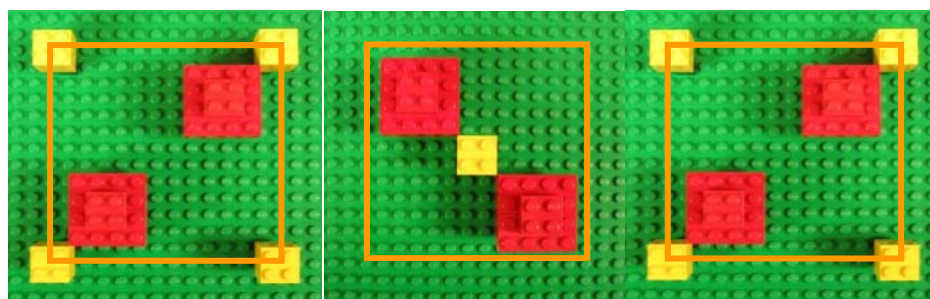


# TiO<sub>2</sub> (rutile form)

LEGO units representing  
ions in this structure:



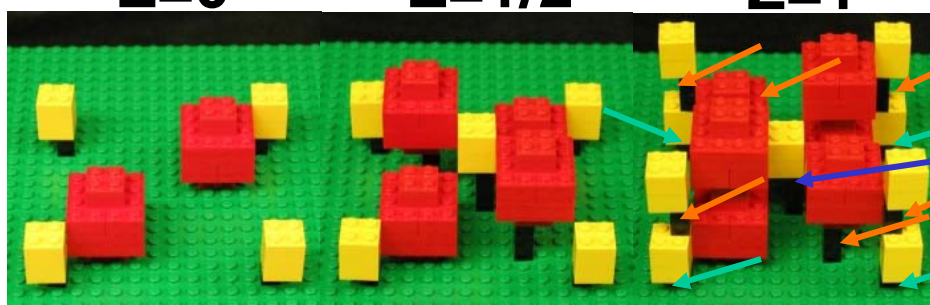
Whole  
ions:



**Z=0**

**Z=1/2**

**Z=1**



These are supports  
made from two 1x1  
bricks (orange)

These are supports  
made from three  
1x1 bricks (blue)

These are supports  
made from one 1x1  
brick (teal)

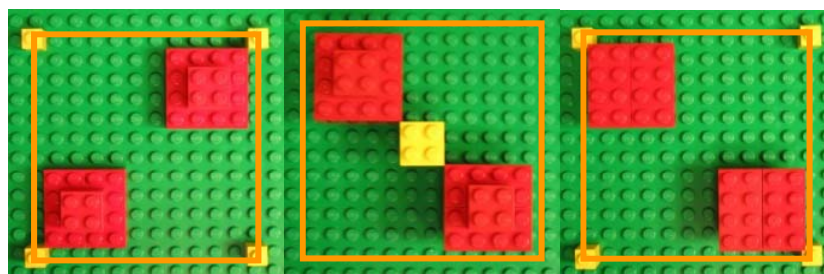
This model Whole ion requires:

17 black 1x1 bricks  
18 yellow 2x2 bricks  
24 red 2x4 bricks  
12 red 2x2 bricks

This model Unit cell requires:

6 yellow 1x1 bricks    16 red 2x4 bricks  
2 yellow 2x2 bricks  
8 black 1x1 bricks  
8 red 2x2 bricks

Unit  
cell:



**Z=0**

**Z=1/2**

**Z=1**

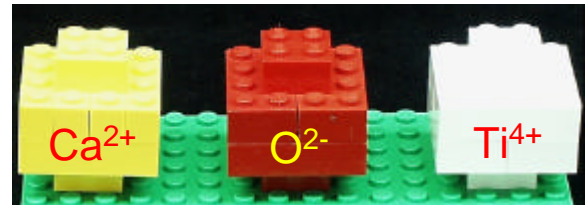


These are supports  
made from two 1x1  
bricks (orange)

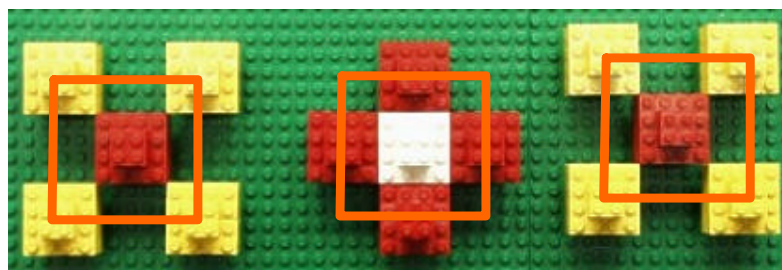


# Perovskite: $\text{CaTiO}_3$

LEGO units  
representing ions  
in this structure:



Whole  
ions:



**Z=0**

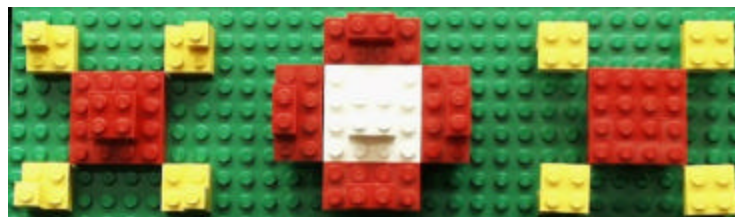
**Z=1/2**

**Z=1**



These are  
supports made  
from four 1x1  
bricks.

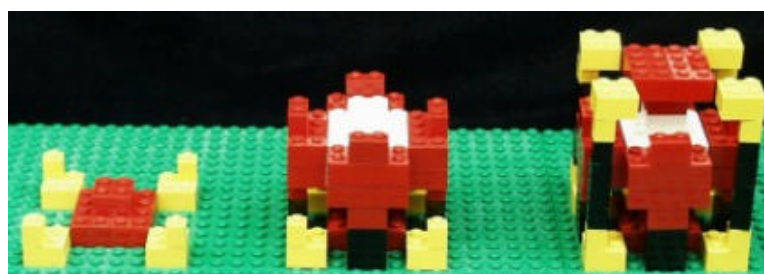
Unit cell:



**Z=0**

**Z=1/2**

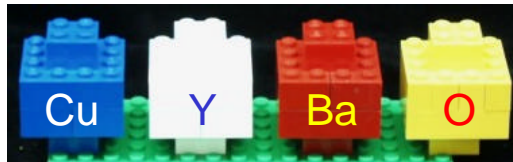
**Z=1**



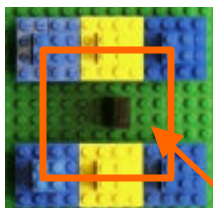


YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>  
(whole ions)

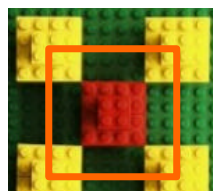
LEGO units representing  
ions in this structure:



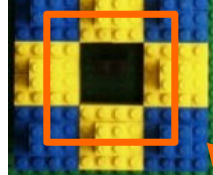
A mixture of  $\text{Cu}^{2+}$  and  $\text{Cu}^{3+}$ ,  $\text{Y}^{3+}$ ,  $\text{Ba}^{2+}$  and  $\text{O}^{2-}$

$$Z=0$$


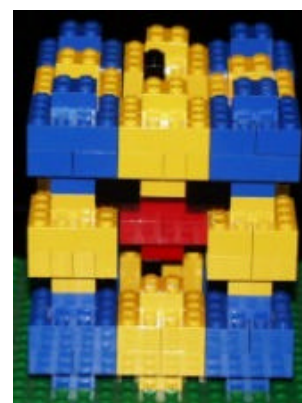
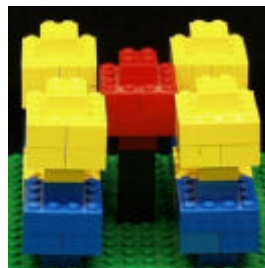
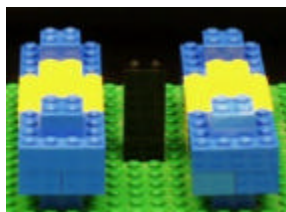
**Z=**  
**0.167**



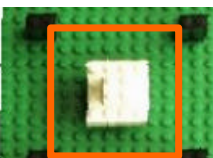
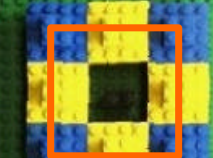
**Z=**  
**0.333**



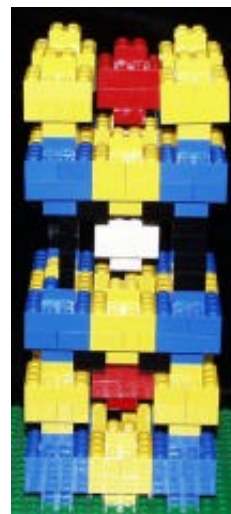
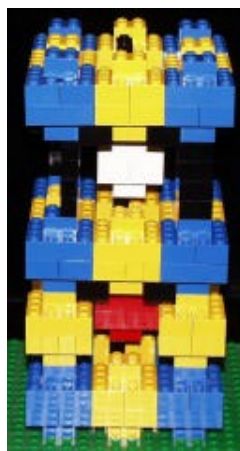
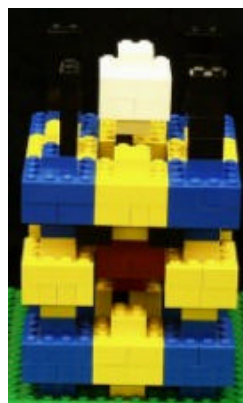
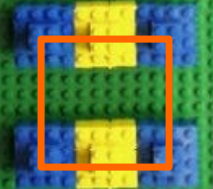
Note: All supports are four 1x2 bricks.



**Z=**  
**0.5**

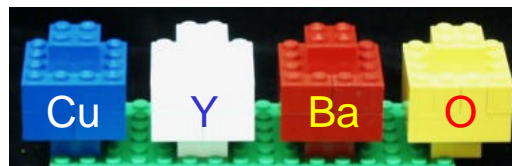

$$Z = 0.667$$


**Z=**  
**0.833**

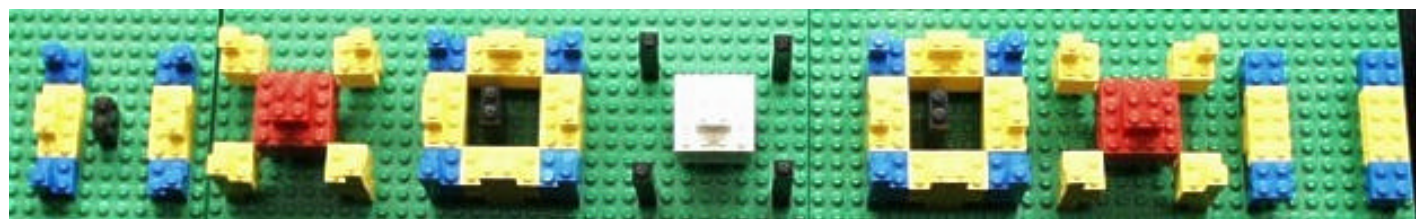

$$Z=1$$


# YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> unit cell

LEGO units representing  
ions in this structure:



Y<sup>3+</sup>, Ba<sup>2+</sup>, O<sup>2-</sup> and a mixture of Cu<sup>2+</sup> and Cu<sup>3+</sup>



Z=0

Z=0.167

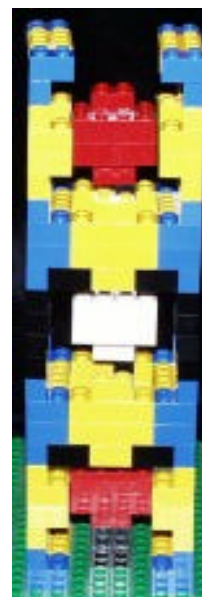
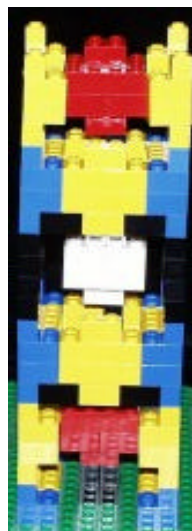
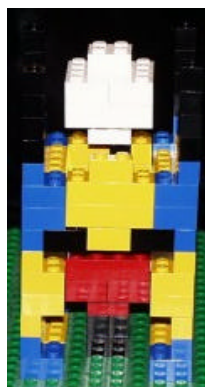
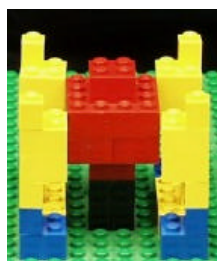
Z=0.333

Z=0.5

Z=0.667

Z=0.833

Z=1



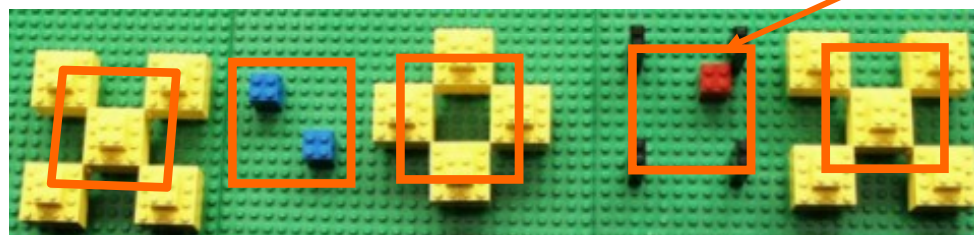


# $\text{Cu}_2\text{HgI}_4$ low temperature phase (whole ions)

LEGO units representing  
ions in this structure:



These are supports  
made from two 1x2  
bricks.



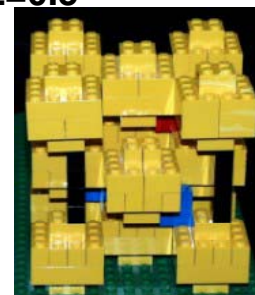
Z=0

Z=0.13

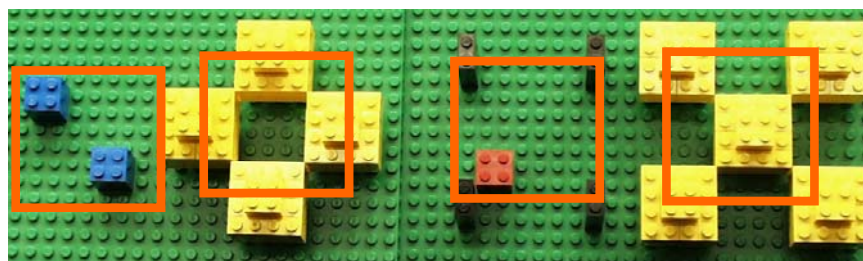
Z=0.25

Z=0.37

Z=0.5



This model requires:  
92 yellow 2x4 bricks  
46 yellow 2x2 bricks  
4 red 2x2 bricks  
8 blue 2x2 bricks  
16 black 2x1 bricks

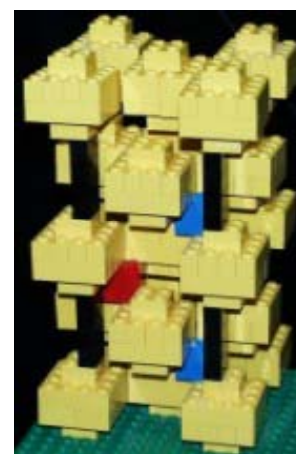
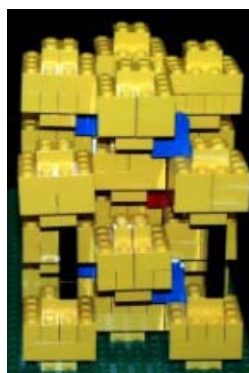


Z=0.63

Z=0.75

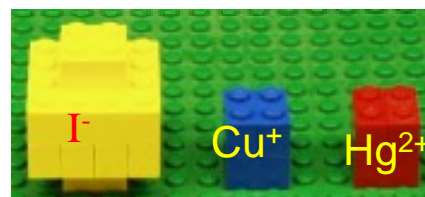
Z=0.87

Z=1



# $\text{Cu}_2\text{HgI}_4$ low temperature phase unit cell

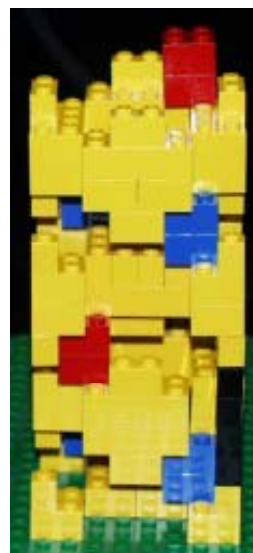
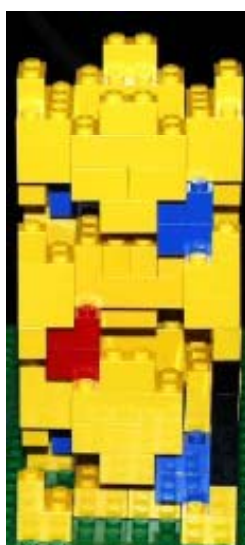
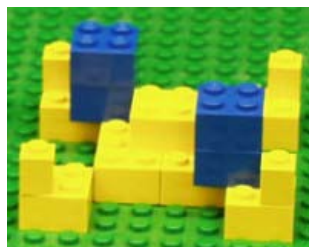
LEGO units representing  
ions in this structure:



**Z=0    Z=0.13    Z=0.25    Z=0.37    Z=0.5    Z=0.63    Z=0.75    Z=0.87    Z=1**

This model requires:

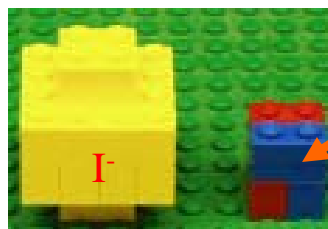
20 yellow 2x4 bricks    4 red 2x2 bricks  
10 yellow 2x2 bricks    8 blue 2x2 bricks  
8 yellow 1x2 bricks    8 yellow 1x1 bricks



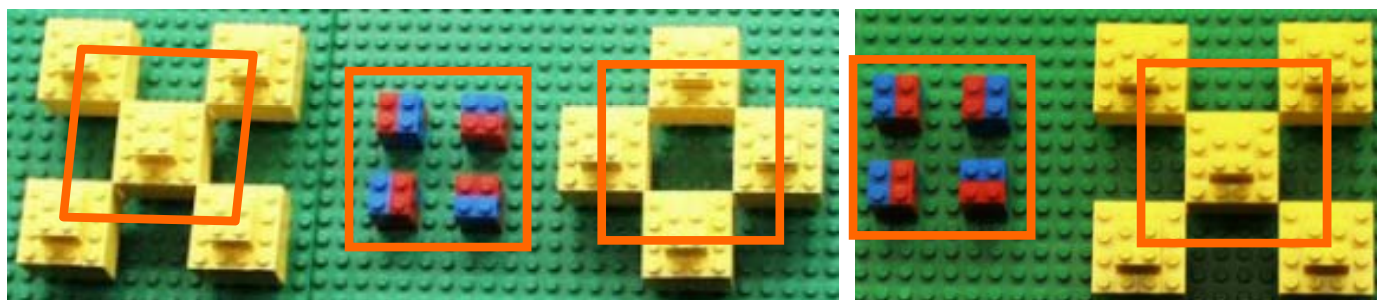


# $\text{Cu}_2\text{HgI}_4$ high temperature phase (whole ions)

LEGO units representing  
ions in this structure:



$\text{Cu}^+, \text{Hg}^{2+}$ ,  
or hole



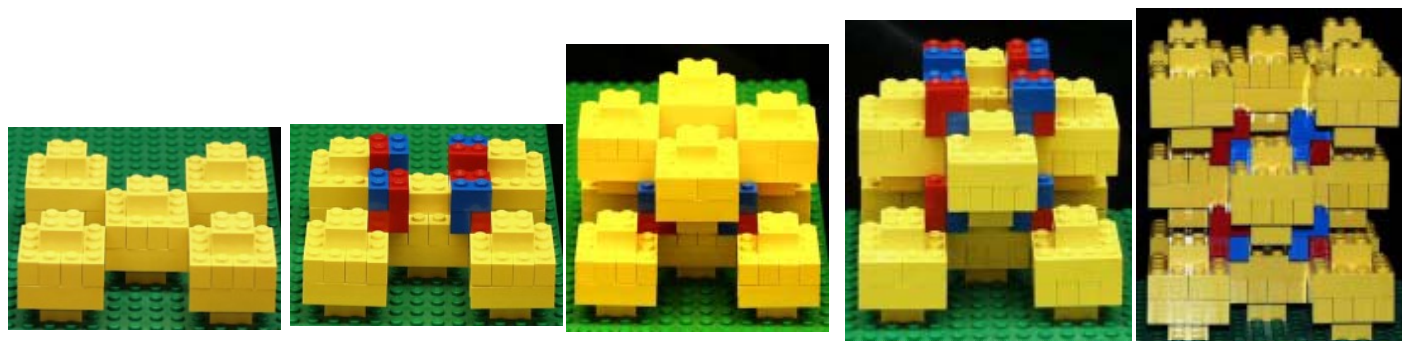
**$Z=0$**

**$Z=1/4$**

**$Z=1/2$**

**$Z=3/4$**

**$Z=1$**



This model requires:

56 yellow 2x4 bricks

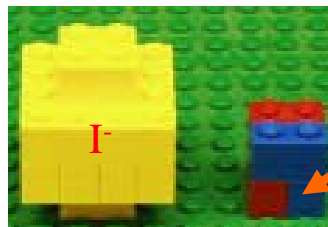
28 yellow 2x2 bricks

16 red 1x2 bricks

16 blue 1x2 bricks

# $\text{Cu}_2\text{HgI}_4$ high temperature phase unit cell

LEGO units representing  
ions in this structure:



$\text{Cu}^+, \text{Hg}^{2+}$ ,  
or hole



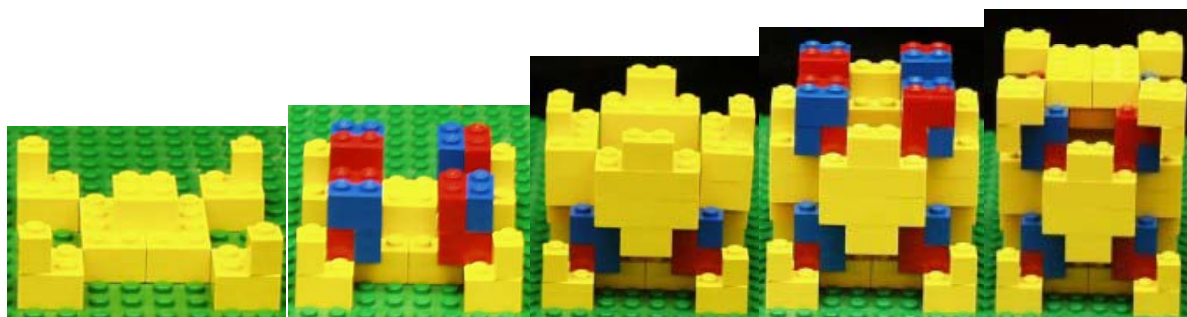
**Z=0**

**Z=1/4**

**Z=1/2**

**Z=3/4**

**Z=1**



This model requires:

12 yellow 2x4 bricks

10 yellow 2x2 bricks

8 yellow 1x2 bricks

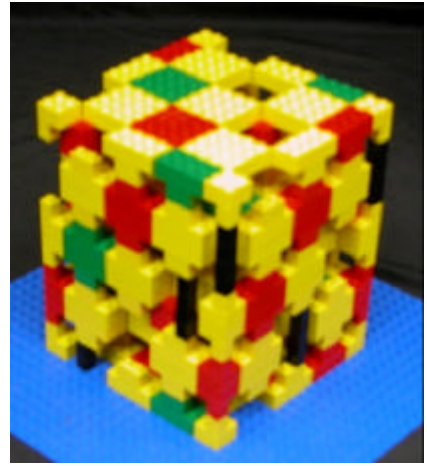
8 yellow 1x1 bricks

16 red 1x2 bricks

16 blue 1x2 bricks

# Magnetite ( $\text{Fe}_3\text{O}_4$ ) Unit Cell

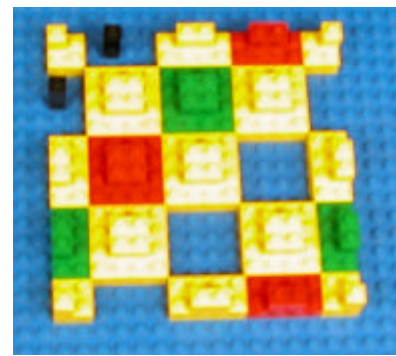
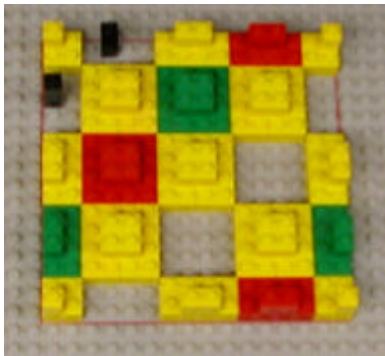
yellow =  $\text{O}^{2-}$ , red =  $\text{Fe}^{3+}$   
green =  $\text{Fe}^{2+}$ , black = spacers



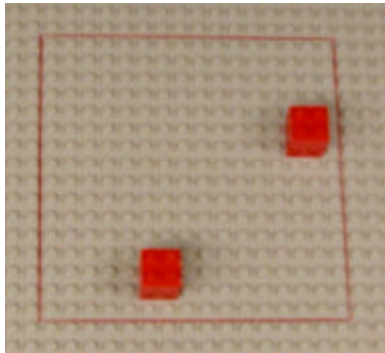
Layer

Build-up

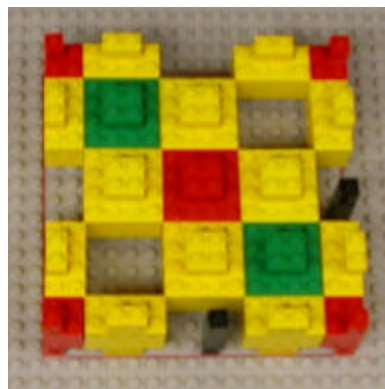
**Z=0**



**Z=0.125**

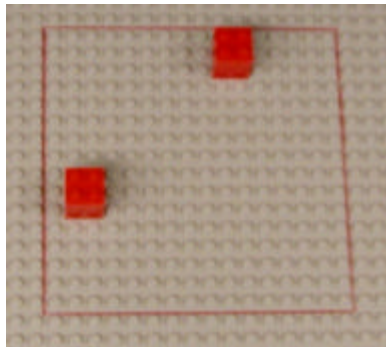


**Z=0.25**

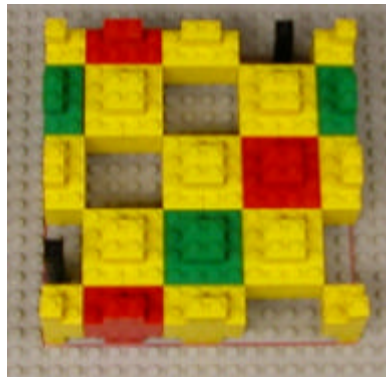




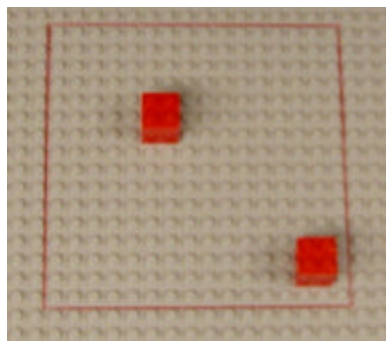
**$Z=0.375$**



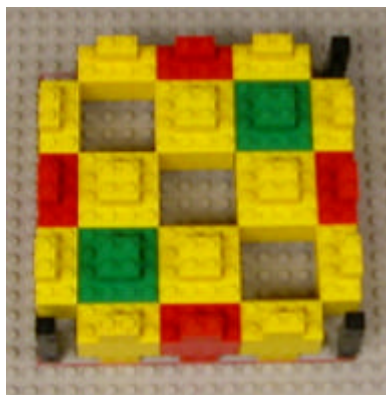
**$Z=0.5$**



**$Z=0.625$**

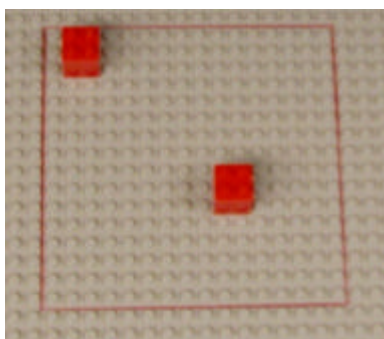


**$Z=0.75$**

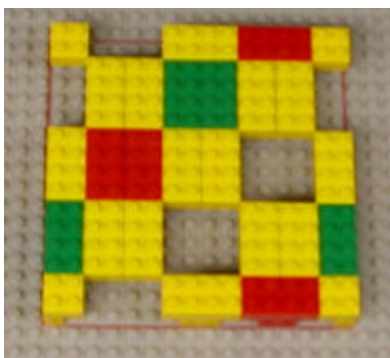




**Z=0.875**



**Z=1**



## Bricks required to build structures

### Partial atoms

Color	Type (pegs)	Number needed
Yellow	2x4	120
	2x2	52
	1x2	48
	1x1	16
Red	2x4	28
	2x2	30
	1x2	16
	1x1	8
Green	2x4	32
	2x2	12
	1x2	8
Black	1x1	32*
Baseboard	16x16	1

### Full atoms (not shown)

Color	Type (pegs)	Number needed
Yellow	2x4	252
	2x2	126
Red	2x4	72
	2x2	52
Green	2x4	52
	2x2	26
Black	1x1	?
Baseboard	18x18	1

\*This is a minimum number. The structure will be more sturdy with more support bricks, but the visibility of the interior of the structure will be diminished.

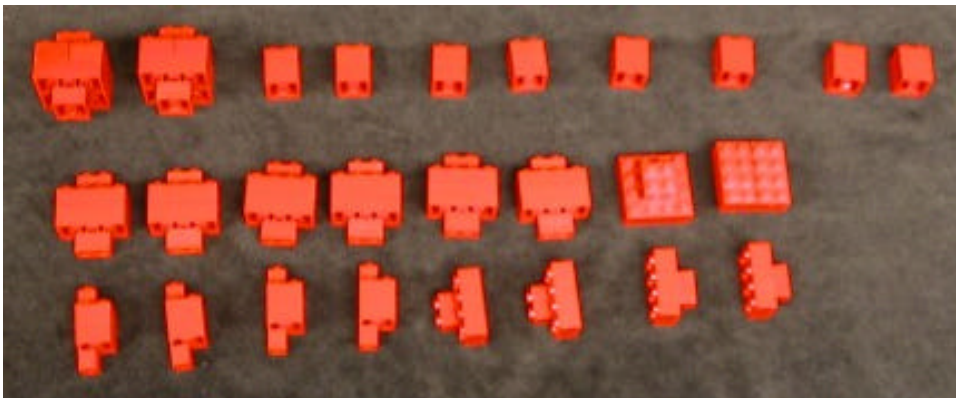
The stoichiometry of magnetite,  $\text{Fe}_3\text{O}_4$ , can be extracted from the unit cell model.

**32 total  $\text{O}^{2-}$  ions**



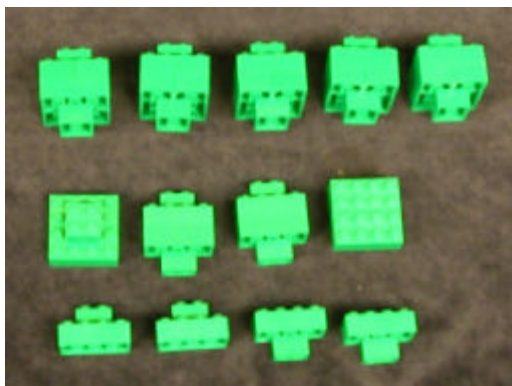
13 whole = 13 ions  
30 half = 15 ions  
12 quarter = 3 ions  
8 eighth = 1 ion  
32 total ions

**16 total  $\text{Fe}^{3+}$  ions**



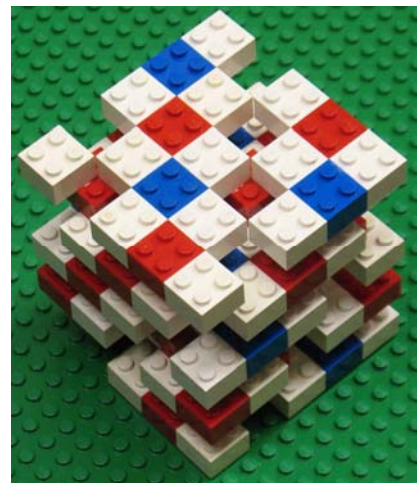
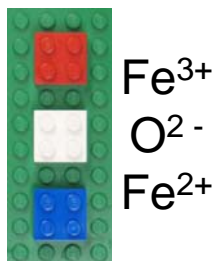
10 whole = 10 ions  
8 half = 4 ions  
8 quarter = 2 ions  
16 total ions

**8 total  $\text{Fe}^{2+}$  ions**



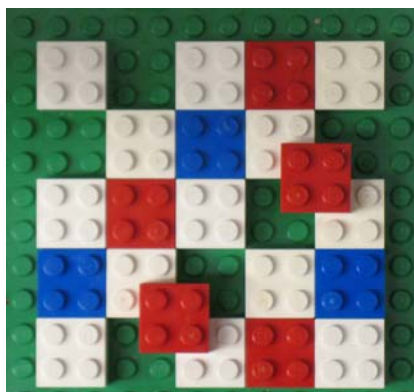
5 whole = 5 ions  
4 half = 2 ions  
4 quarter = 1 ions  
8 total ions

# Magnetite ( $\text{Fe}_3\text{O}_4$ ) whole small atoms

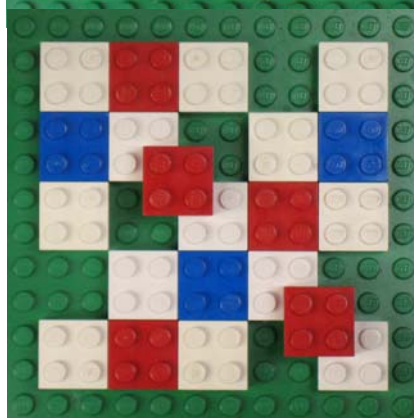


## Layer Sequence

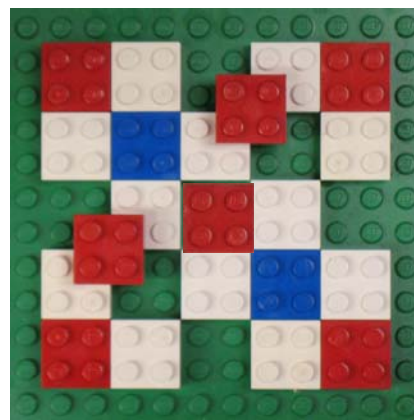
**Z = 0  
& 0.125**



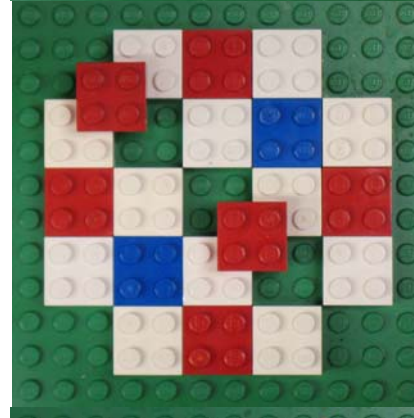
**Z = 0.5  
& 0.625**



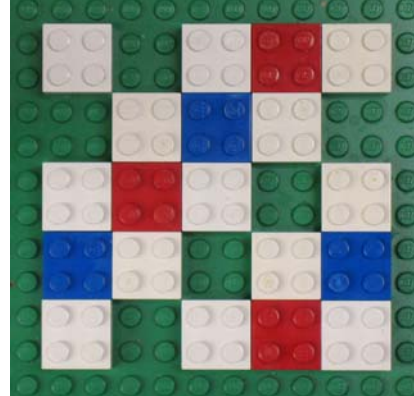
**Z = 0.25  
& 0.375**



**Z = 0.75  
& 0.875**



**Z = 1**



This model requires:

26 red 2x2 bricks

63 white 2x2 bricks

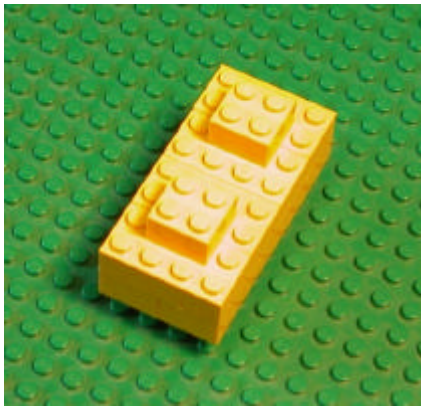
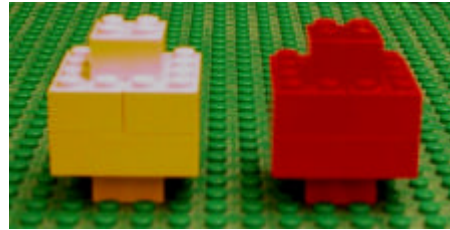
13 blue 2x2 bricks

\*\*\*If glued, no support necessary

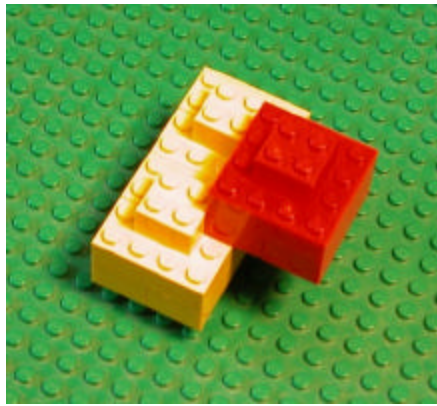


# NiTi Low Temperature Martensite Phase (whole atoms; small cell)

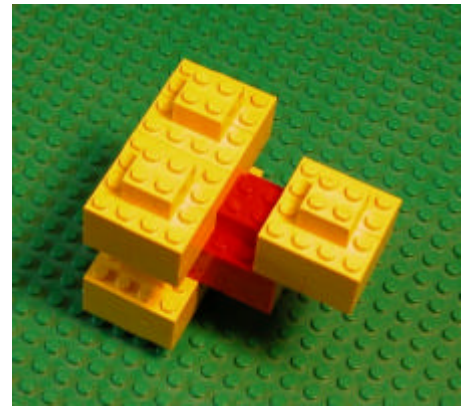
LEGO unit representing  
atoms in this structure:  
(Different colors represent  
different elements.)



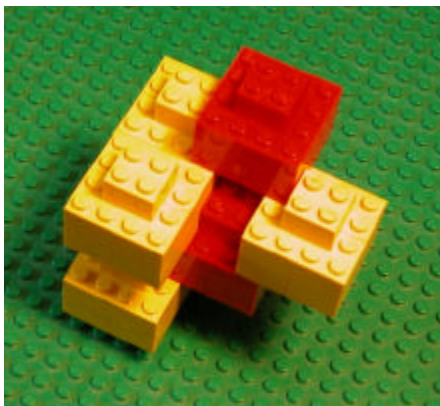
**Step 1**



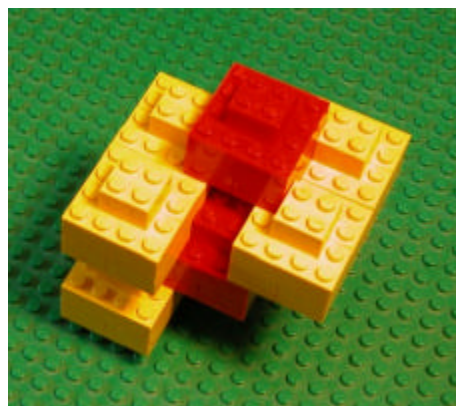
**Step 2**



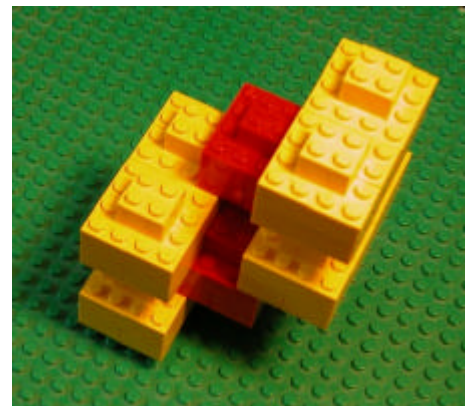
**Step 3**



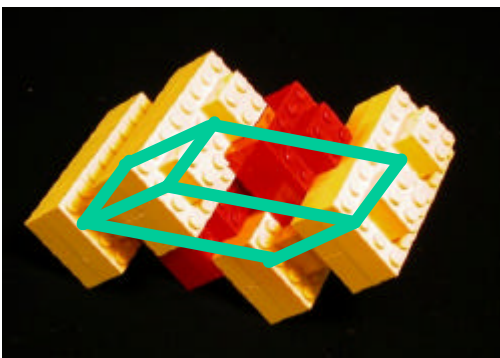
**Step 4**



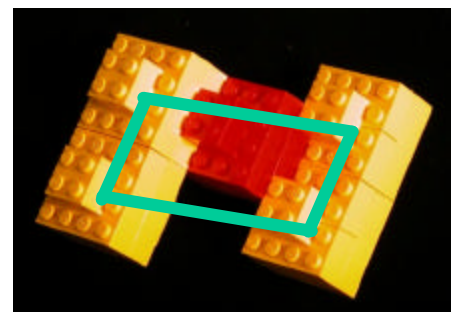
**Step 5**



**Step 6**



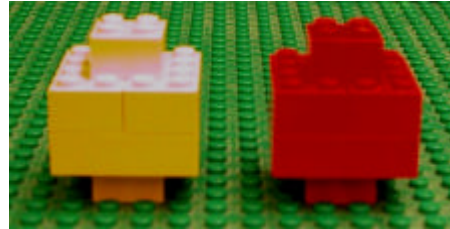
Lines represent  
approximate  
boundaries of the  
unit cell.



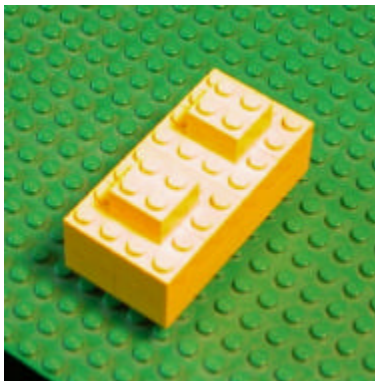
Layers:  $Z = 0,1$

# NiTi Low Temperature Martensite Phase (whole atoms; large cell)

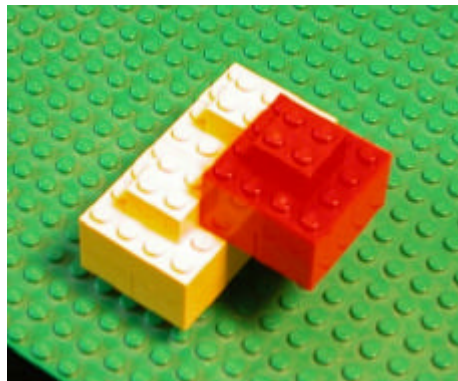
LEGO unit representing  
atoms in this structure:  
(Different colors represent  
different elements.)



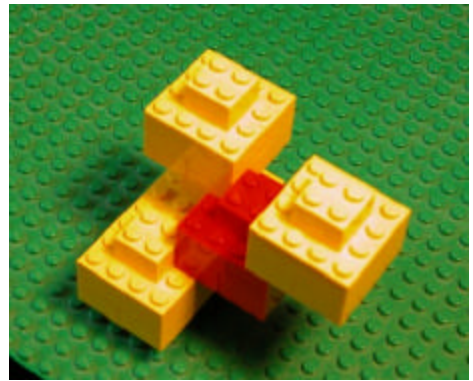
NOTE: The unit cell represented by this structure has atoms that are not parallel to the bottom face of the unit cell. The structure may be built in the following series of steps and then later tilted.



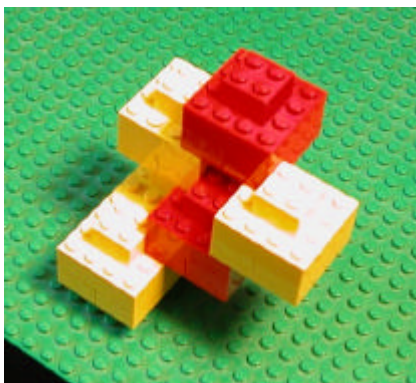
**Step 1**



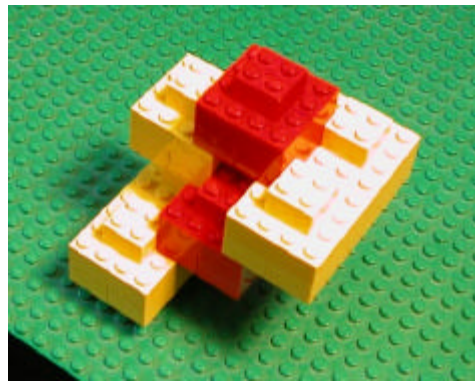
**Step 2**



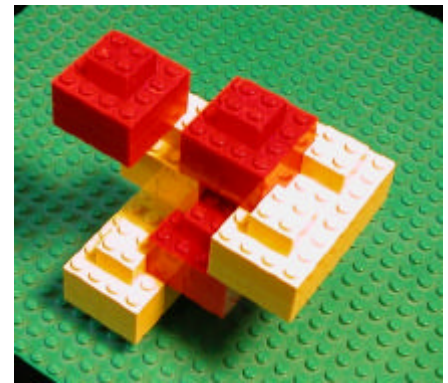
**Step 3**



**Step 4**

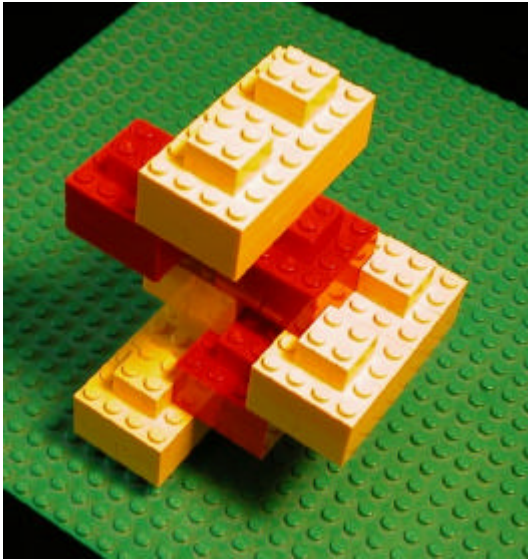


**Step 5**

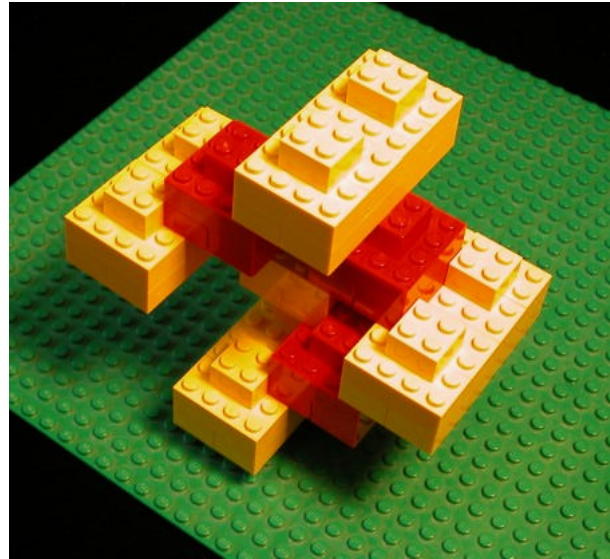


**Step 6**



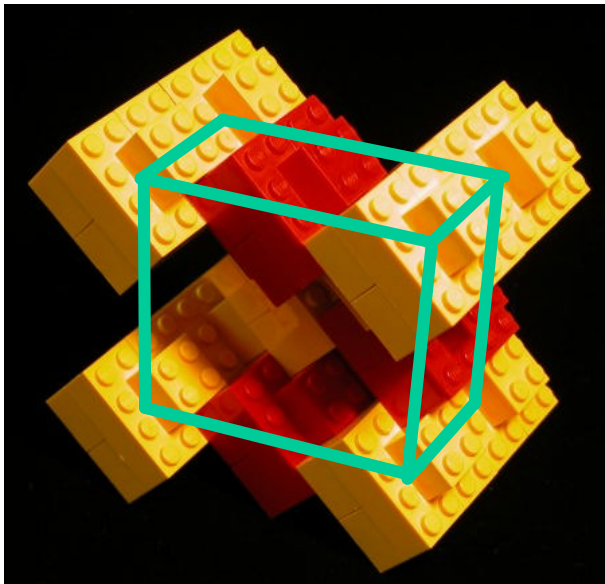


**Step 7**



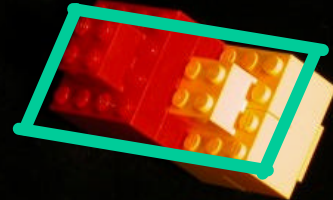
**Step 8**

Lines represent approximate boundaries of the unit cell.

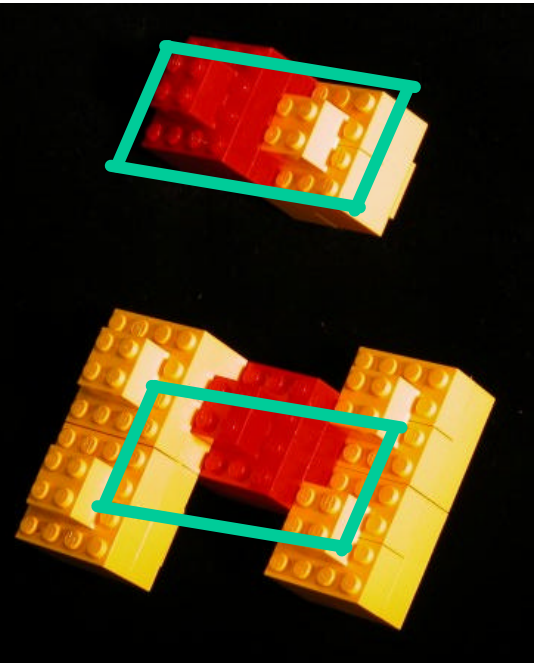


Layers:

$$Z = \frac{1}{2}$$



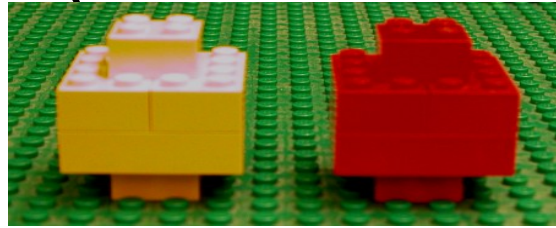
$$Z = 0, 1$$





# NiTi High Temperature Austenite Phase (whole atoms)

LEGO unit representing atoms in this structure:  
(Different colors represent different elements.)



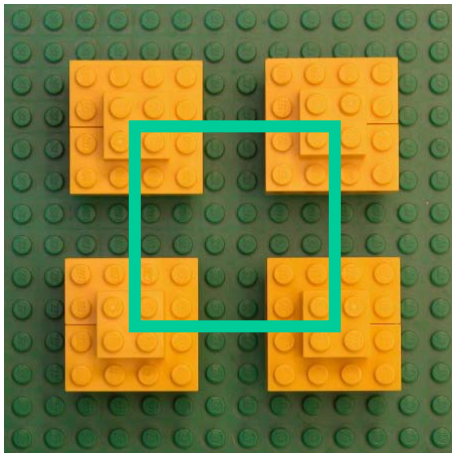
This model requires:

32 yellow 2x4 bricks

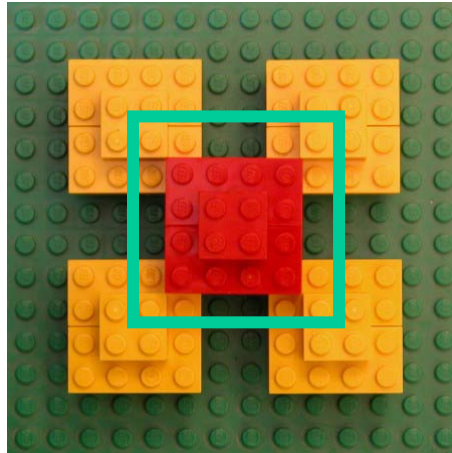
16 yellow 2x2 bricks

4 red 2x4 bricks

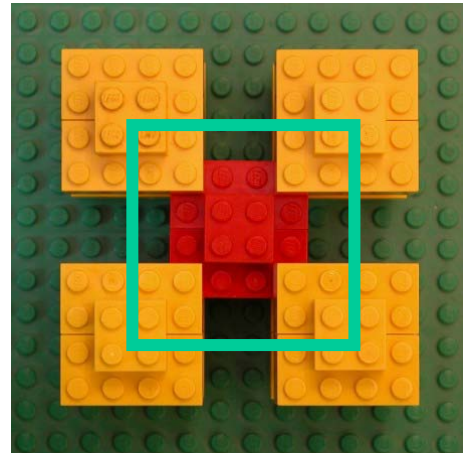
2 red 2x2 bricks



**Z=0**

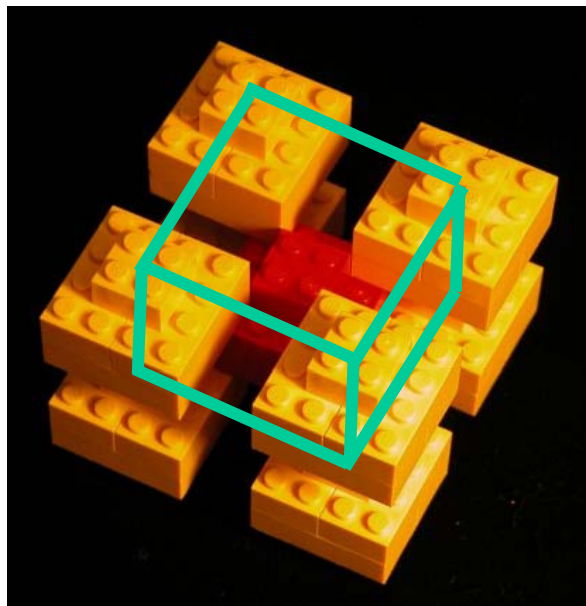


**Z=1/2**



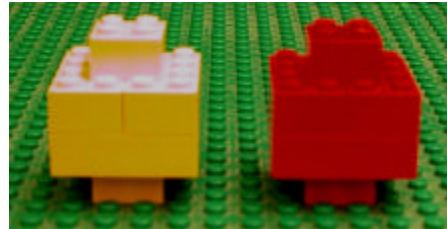
**Z=1**

Lines represent  
approximate  
boundaries of the  
unit cell.

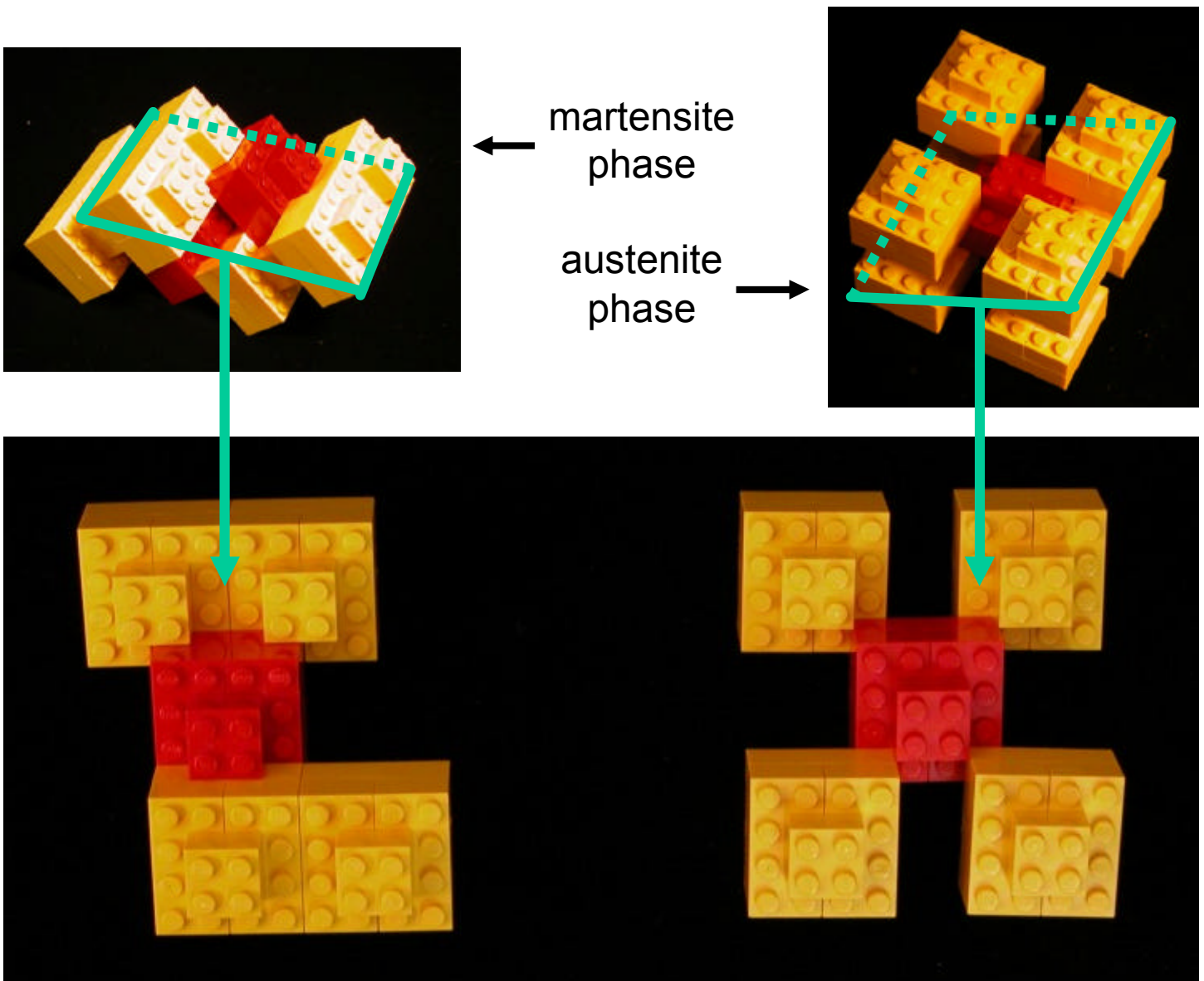


# NiTi Low Temperature Martensite Phase vs. High Temperature Austenite Phase

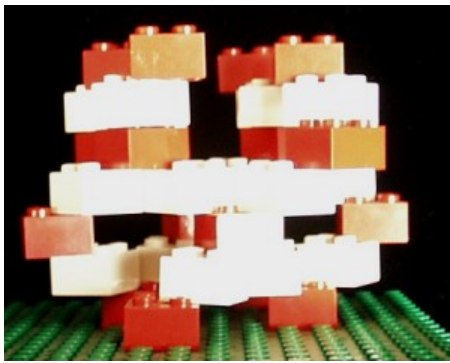
LEGO unit representing  
atoms in this structure:  
(Different colors represent  
different elements.)



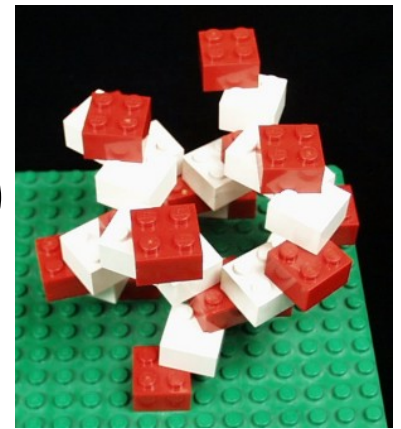
The structures can be represented as planes of Ni and Ti atoms.  
The lines represent the planes of atoms.





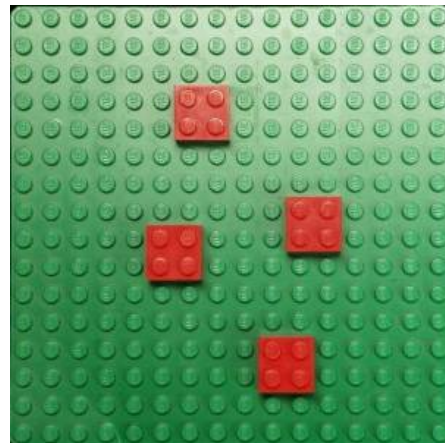
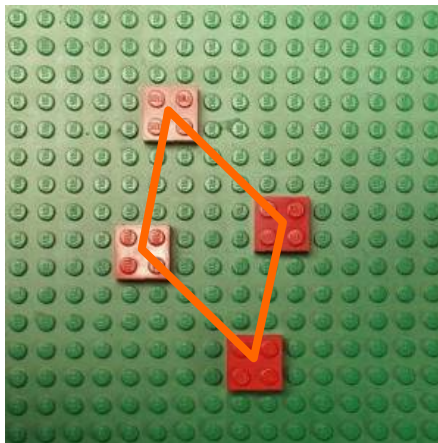


# Quartz (whole atoms)

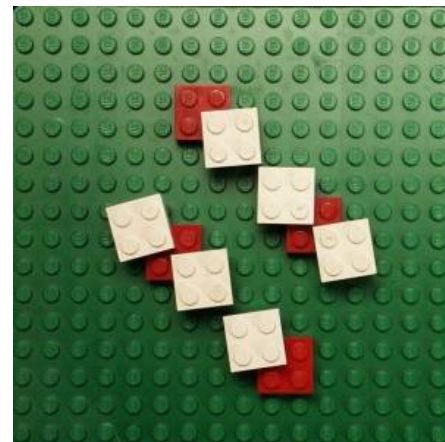
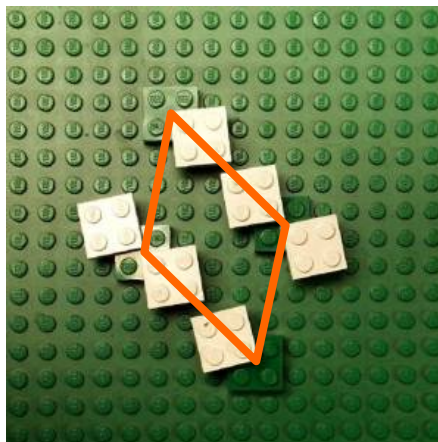


red = Si    white = O

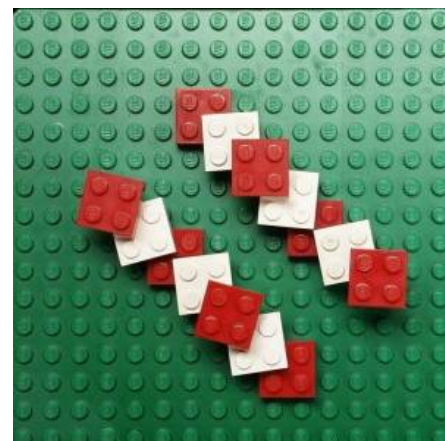
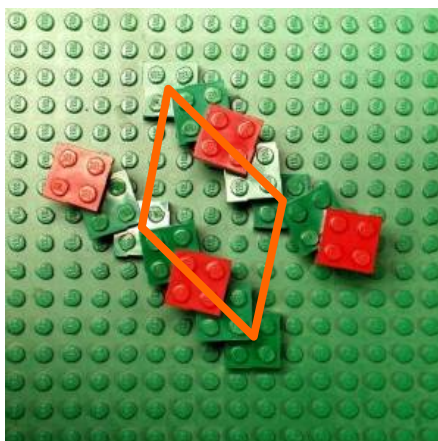
**Z=**  
**0,1**



**Z=**  
**0.167,**  
**0.833**

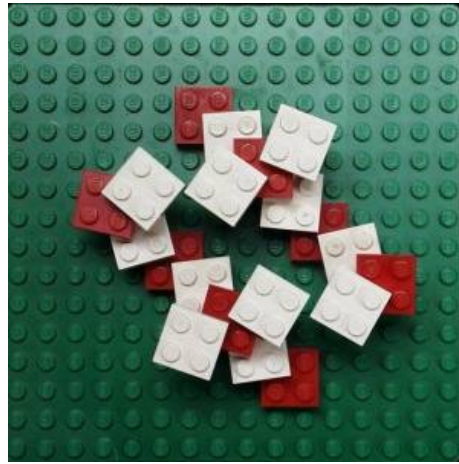
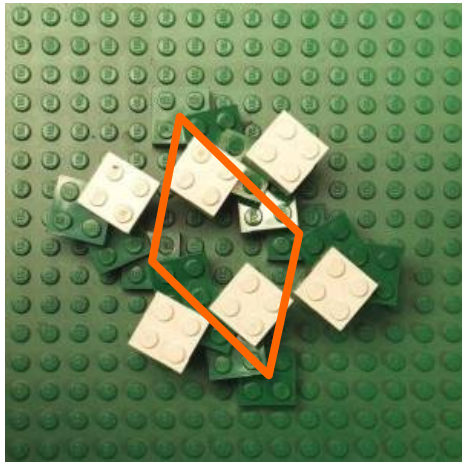


**Z=**  
**0.333,**  
**0.667**

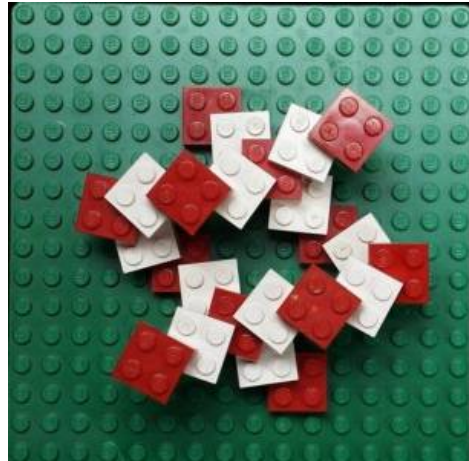
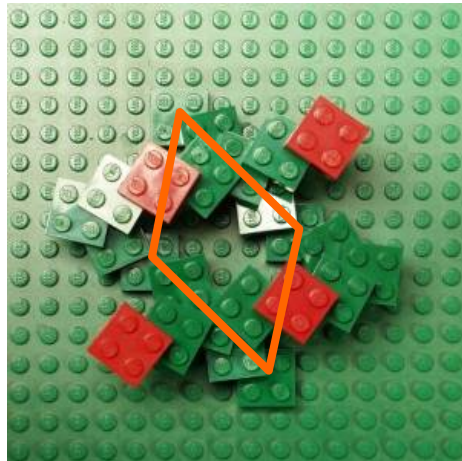




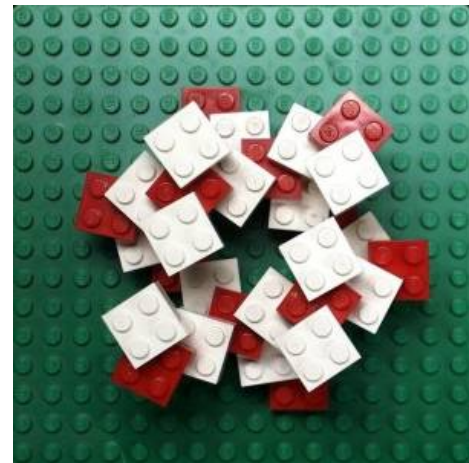
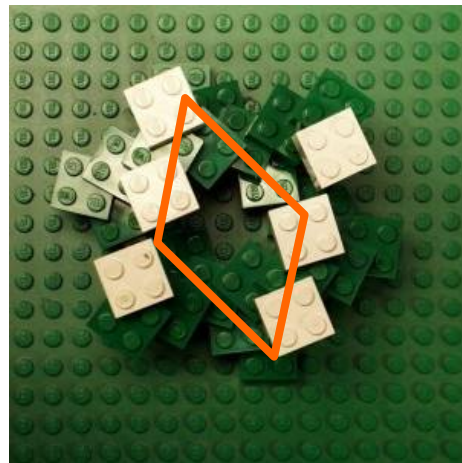
**Z=**  
**0.5**



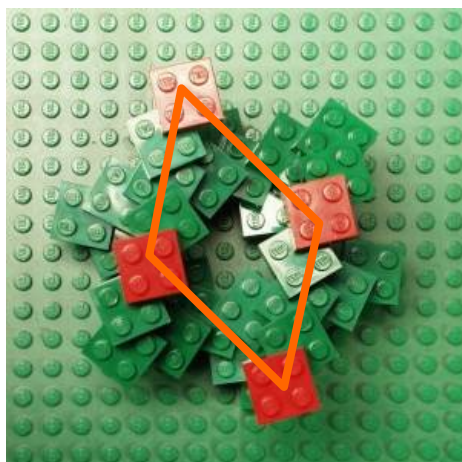
**Z=**  
**0.333,**  
**0.667**



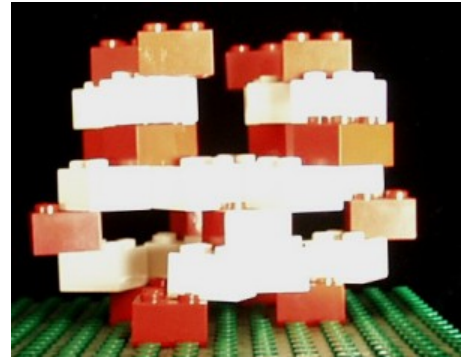
**Z=**  
**0.167,**  
**0.833**



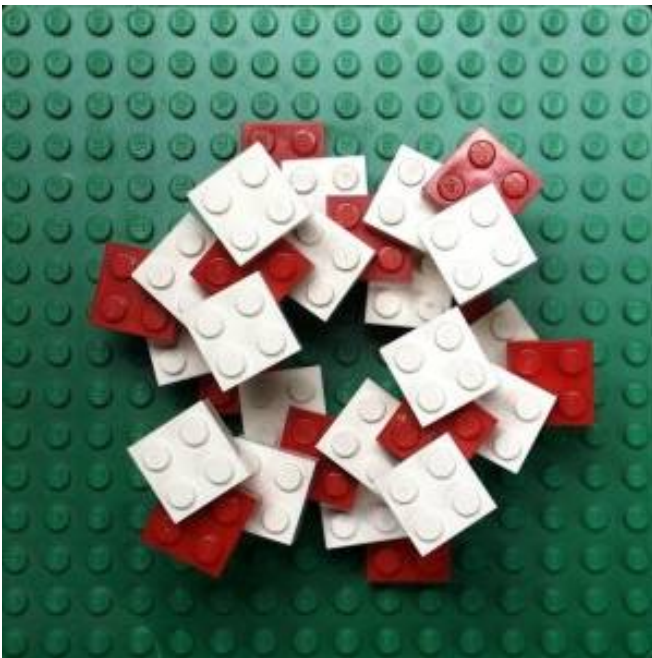
**Z=**  
**0,1**



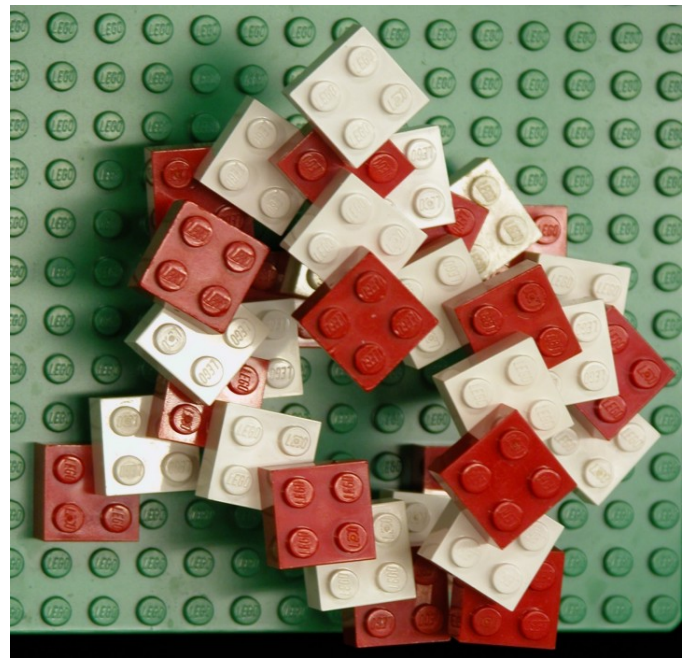
# Crystalline vs. Amorphous Quartz (whole atoms)



red = Si    white = O



Crystalline



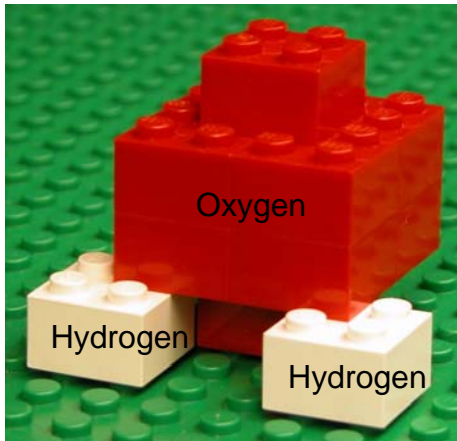
Amorphous

Note in both structures that the rules for bonding are the same: each Si atom is attached to four O atoms and each O atom is attached to two Si atoms. However, the atoms are organized in three-dimensional patterns in the crystalline phase. In the amorphous (glassy) phase, that order is not present. The atoms in the amorphous phase show a liquid-like disorder, yet they do not move about and the material is a solid.



# Ice Ih (typical phase) (whole atoms)

LEGO® unit representing  
 $\text{H}_2\text{O}$  in this structure:



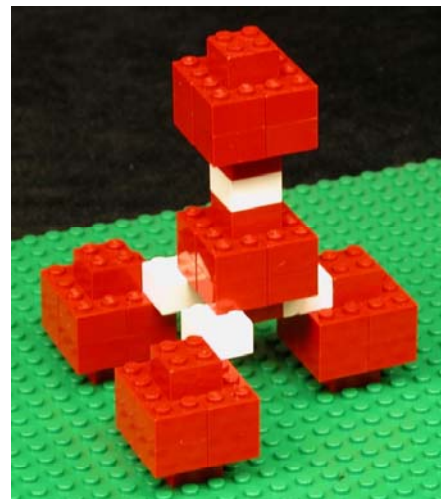
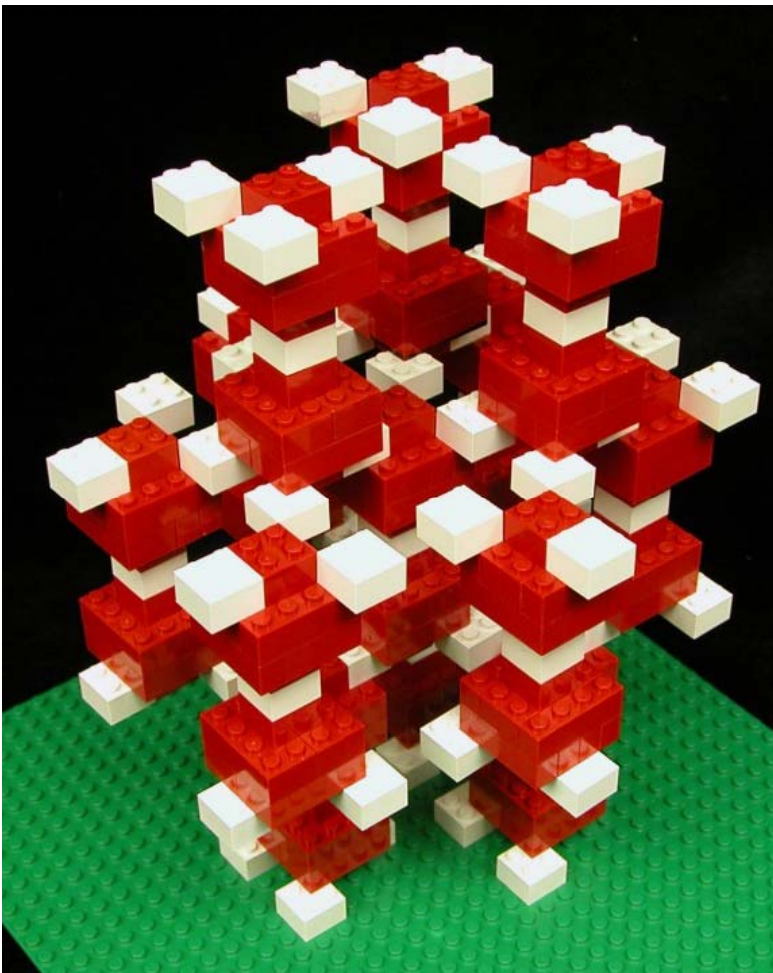
The oxygen atoms are connected to the other oxygen atoms in a tetrahedral geometry via covalent and hydrogen bonds to hydrogen atoms. Note in this representation the hydrogen atoms are shown as equally distant from the oxygen atoms that they bridge. In reality, the hydrogen atoms are closer to the oxygen atoms to which they are covalently bonded and further from the oxygen atoms to which they are hydrogen bonded.

This model requires:

73 white 2x2 bricks

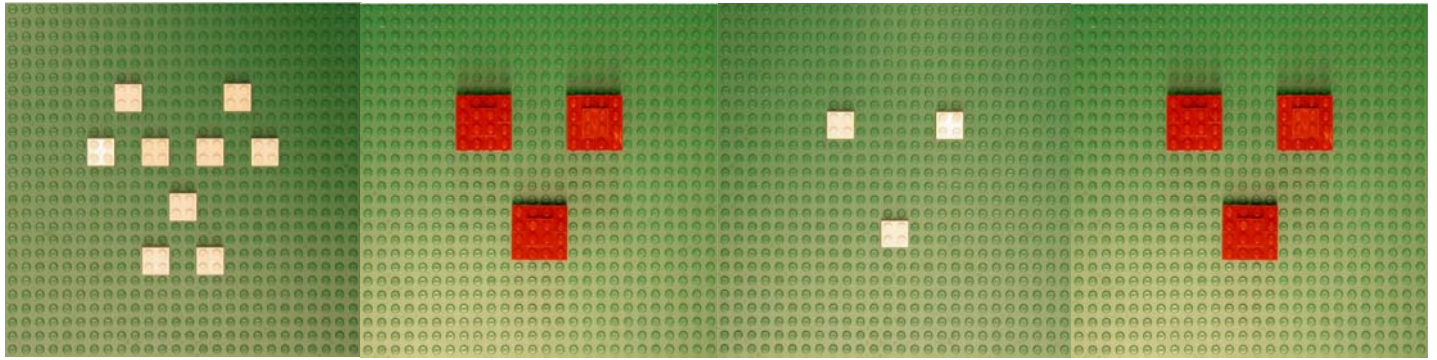
104 red 2x4 bricks

52 red 2x2 bricks



Angle view of the Ice Ih structure  
(The relative oxygen atom positions  
are similar to the lonsdaleite  
structure.)



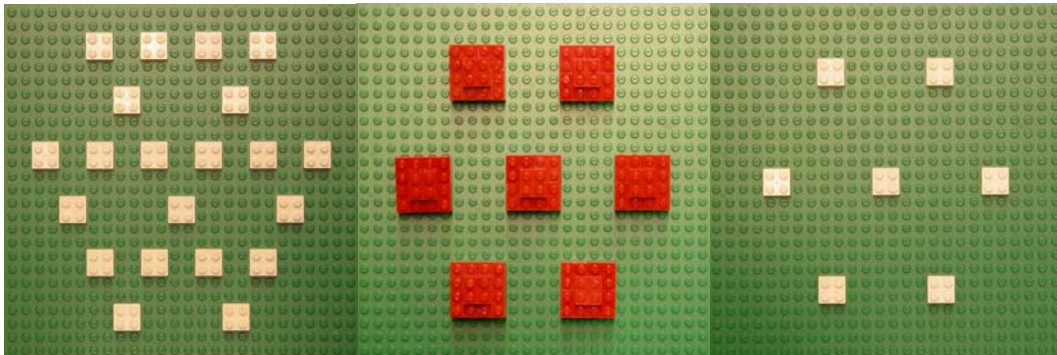


**Layer 1  
(bottom)**

**Layer 2**

**Layer 3**

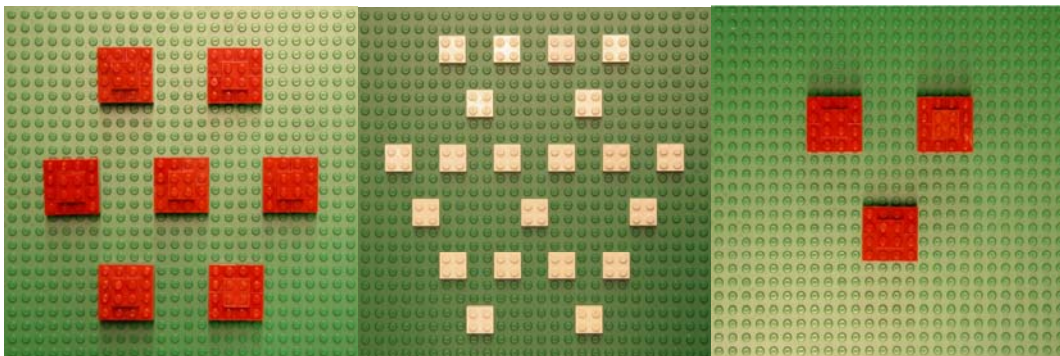
**Layer 4**



**Layer 5**

**Layer 6**

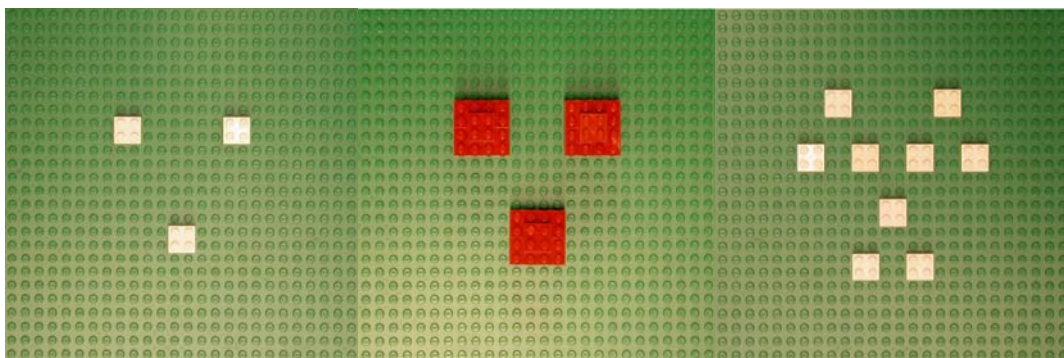
**Layer 7**



**Layer 8**

**Layer 9**

**Layer 10**



**Layer 11**

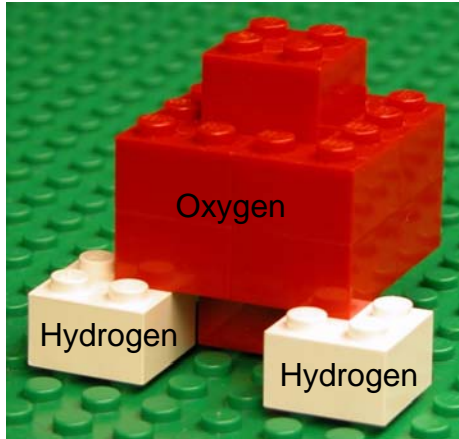
**Layer 12**

**Layer 13  
(top)**



# Ice Ic (a low-temperature phase) (whole atoms)

LEGO® unit representing  
 $\text{H}_2\text{O}$  in this structure:



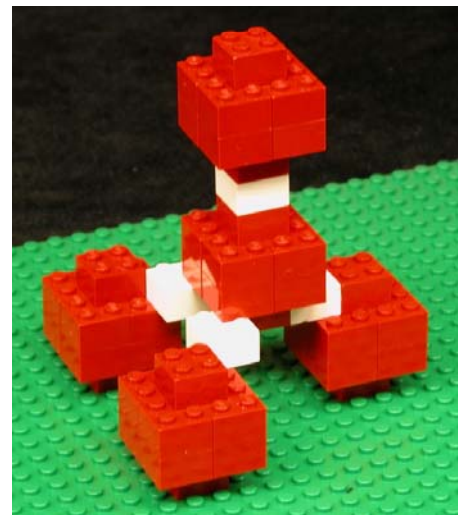
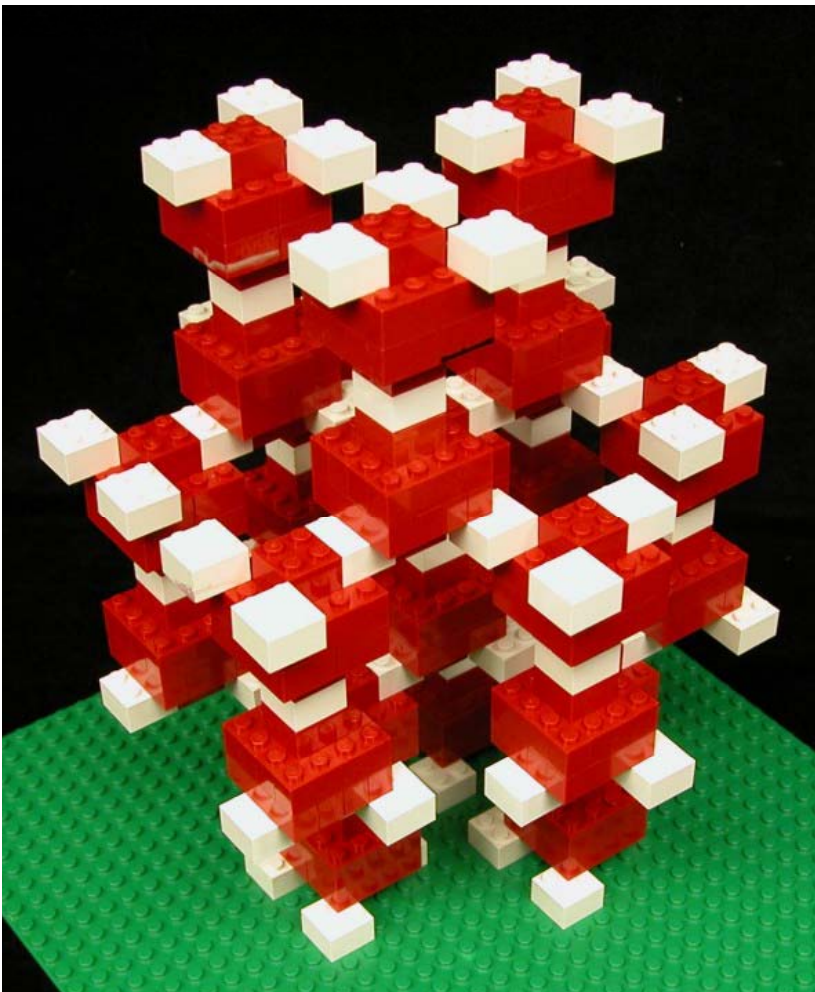
The oxygen atoms are connected to the other oxygen atoms in a tetrahedral geometry via covalent and hydrogen bonds to hydrogen atoms. Note in this representation the hydrogen atoms are shown as equally distant from the oxygen atoms that they bridge. In reality, the hydrogen atoms are closer to the oxygen atoms to which they are covalently bonded and further from the oxygen atoms to which they are hydrogen bonded.

This model requires:

73 white 2x2 bricks

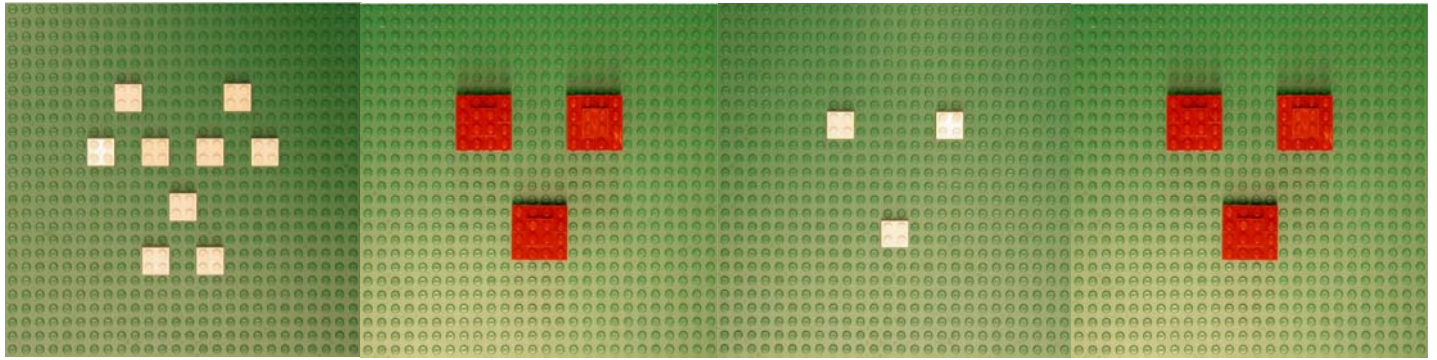
104 red 2x4 bricks

52 red 2x2 bricks



Angle view of the Ice Ic structure  
(The relative oxygen atom positions  
are similar to the diamond structure.)



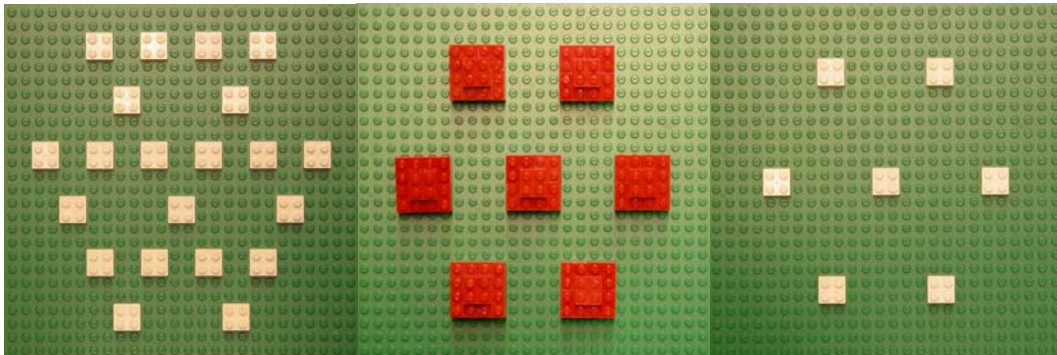


**Layer 1  
(bottom)**

**Layer 2**

**Layer 3**

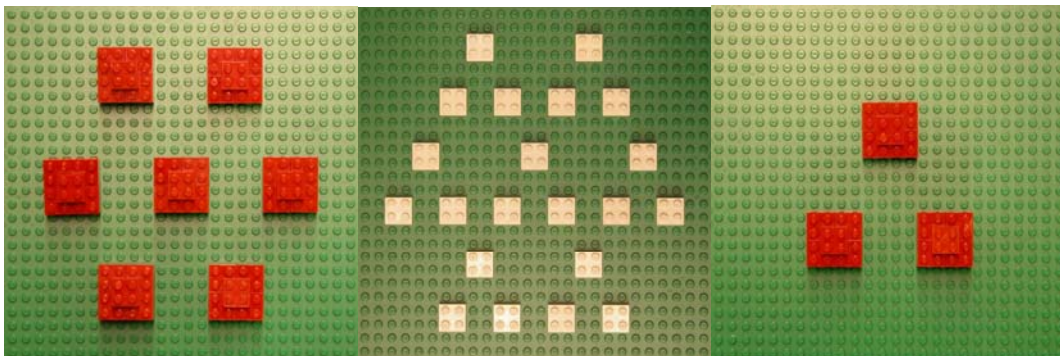
**Layer 4**



**Layer 5**

**Layer 6**

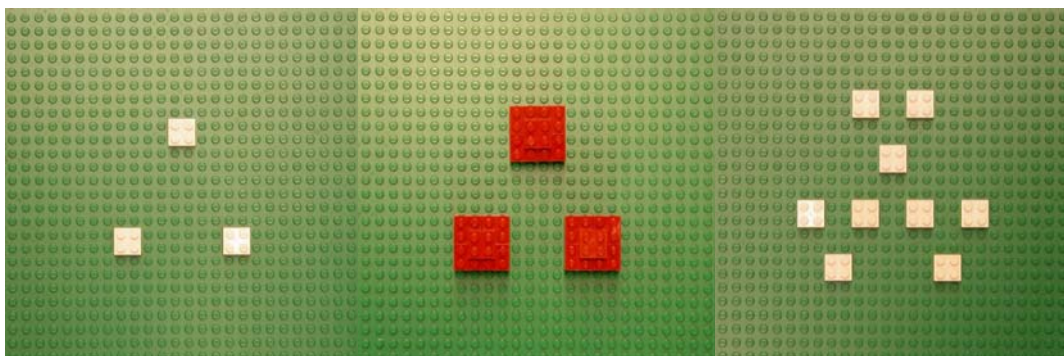
**Layer 7**



**Layer 8**

**Layer 9**

**Layer 10**



**Layer 11**

**Layer 12**

**Layer 13  
(top)**

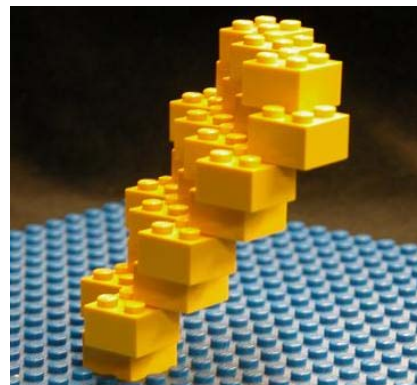
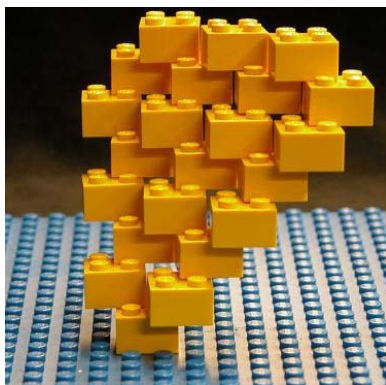
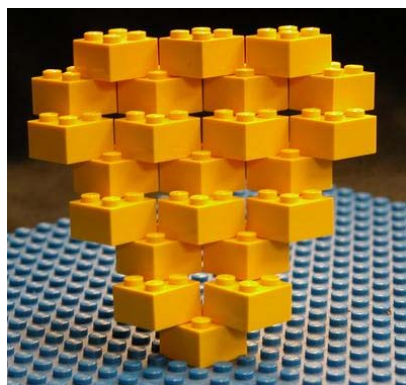


# Arsenic (whole atoms)

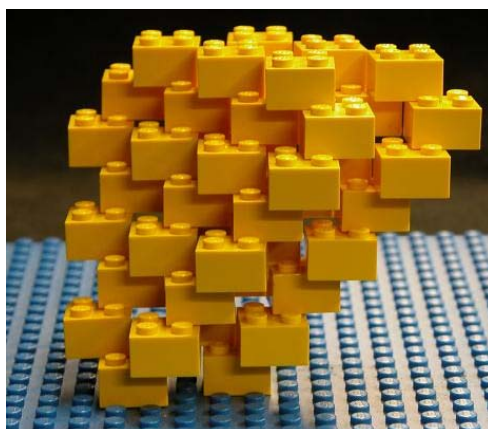
LEGO unit representing  
atoms in this structure:



One layer – sheet of hexagons



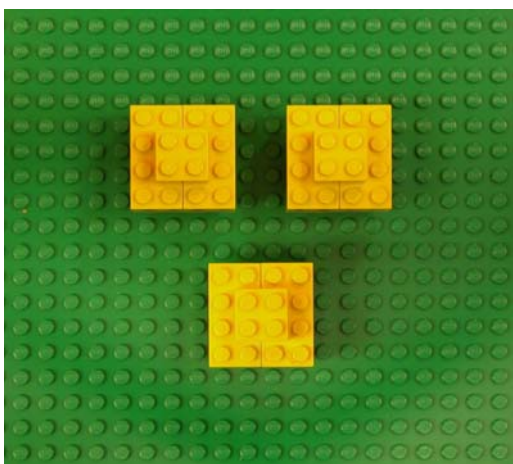
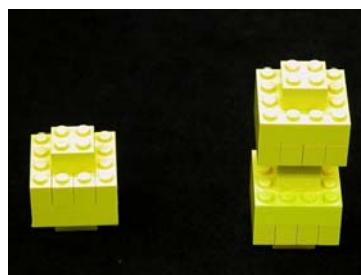
Two layers



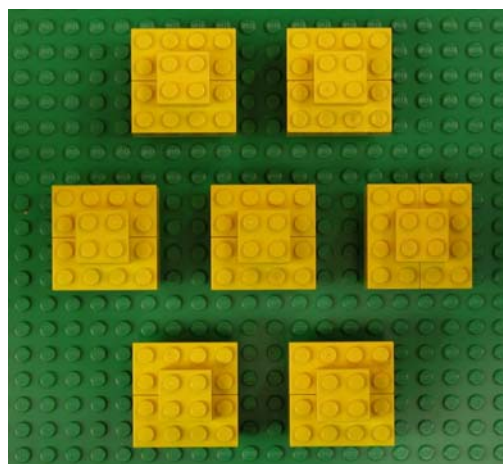
This model requires:  
44 yellow 2x2 bricks

# Nitrogen (whole atoms)

LEGO unit representing  
atoms in this structure:

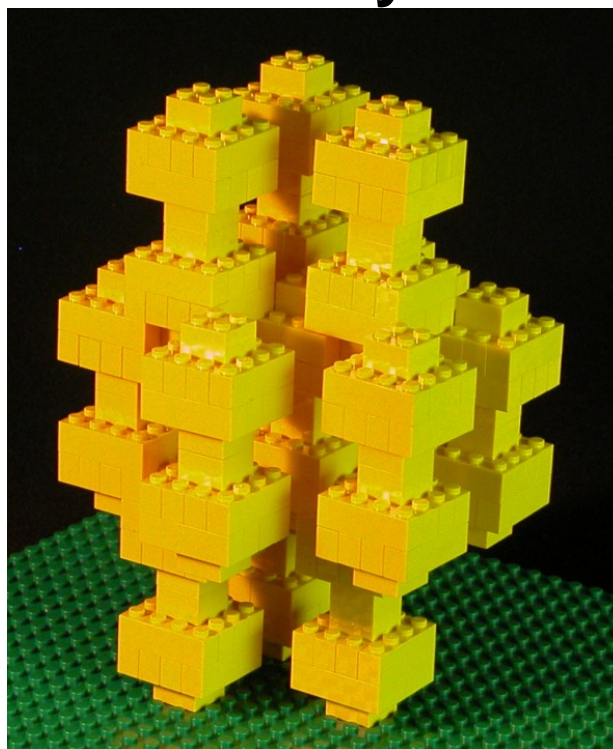


“A” Layer



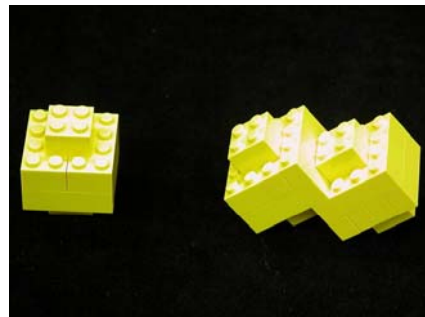
“B” Layer

Angle view of nitrogen structure  
(Layers **ABABABA...**):



# Iodine Structure (whole atoms)

LEGO unit representing  
atoms in this structure:



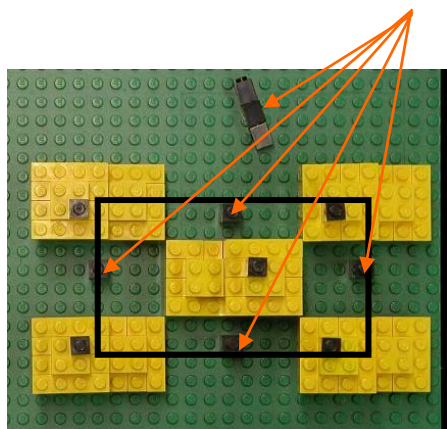
This model requires:

112 yellow 2x4 bricks

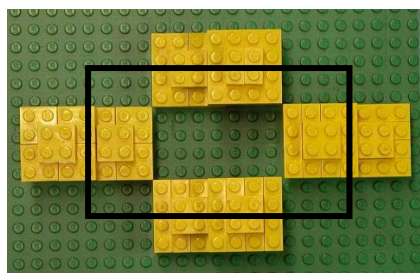
56 yellow 2x2 bricks

20 black 1x1 bricks

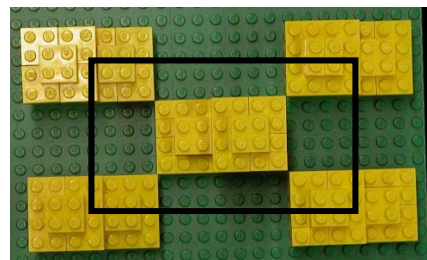
These are supports made  
from three 1x1 bricks.



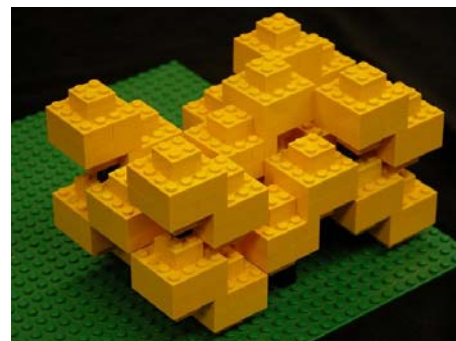
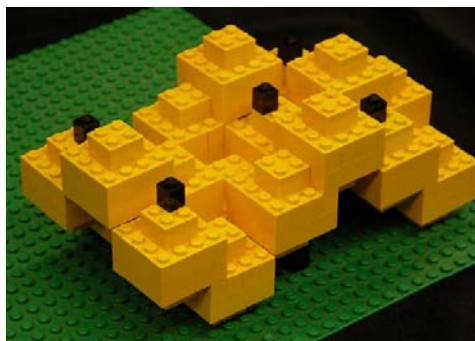
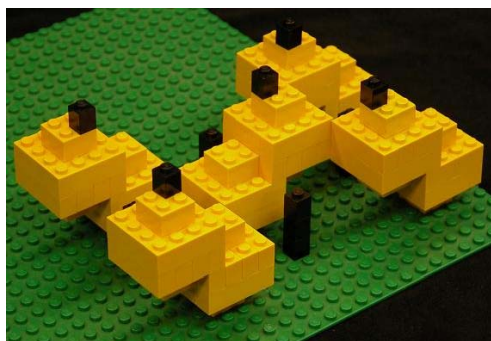
**Z=0**



**Z=1/2**



**Z=1**





# Phosphorus (whole atoms)

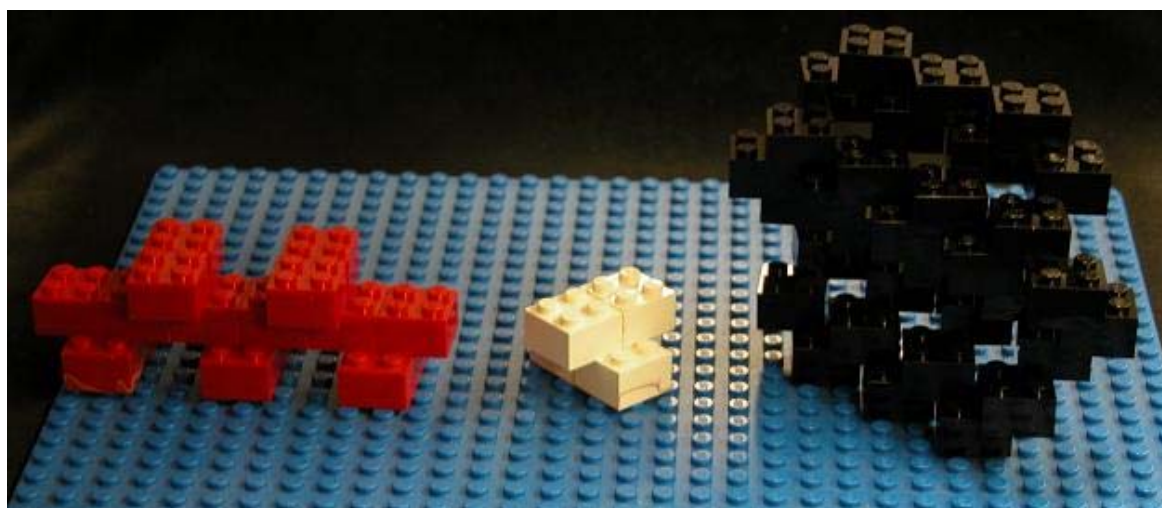
LEGO unit representing  
atoms in this structure:



Red Allotrope

White Allotrope

Black Allotrope

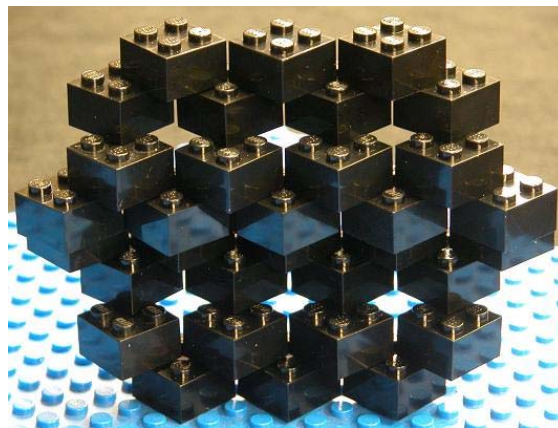
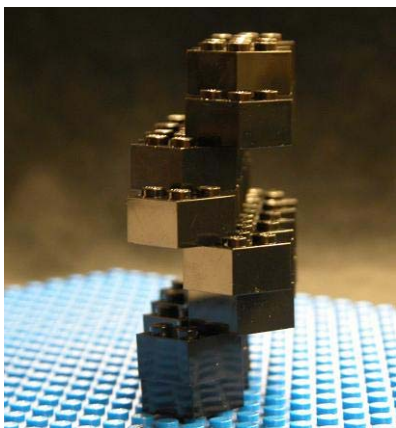


Chains of four-  
atom groups

Four-atom  
group

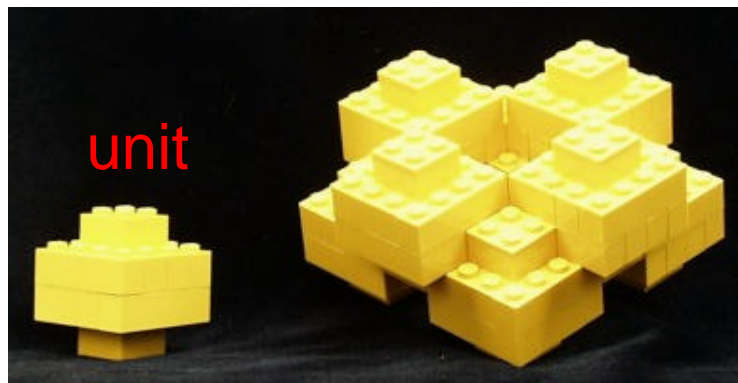
Rippled sheets  
of hexagons

Black phosphorus detail

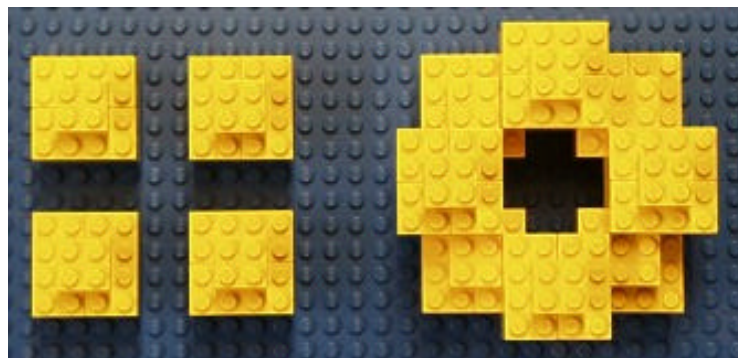


# Sulfur (whole atoms)

## Rhombic/Orthorhombic Sulfur

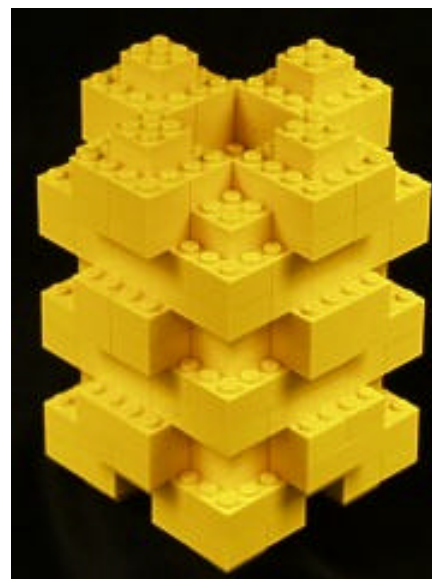


### Build Up Sequence



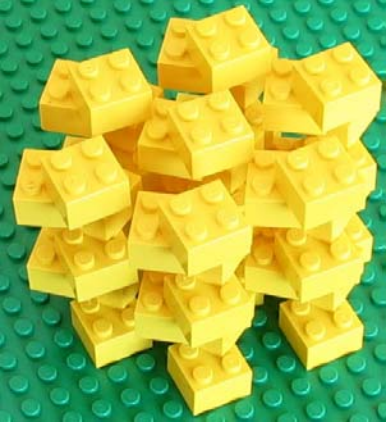
Level 1

Level 2



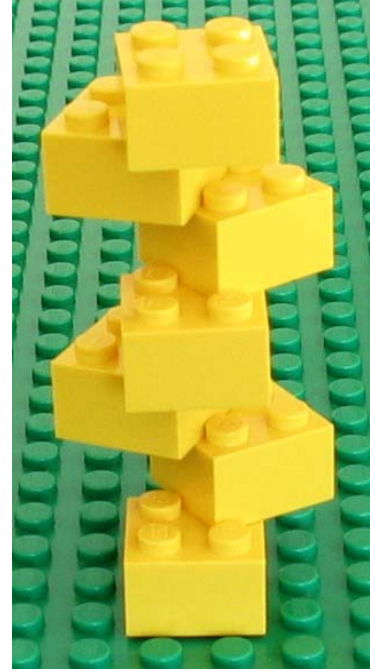
## Monoclinic Sulfur





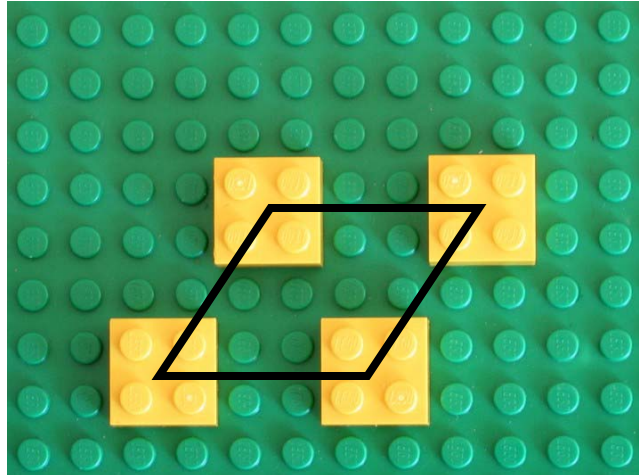
yellow = Se

# Trigonal Selenium (whole atoms)

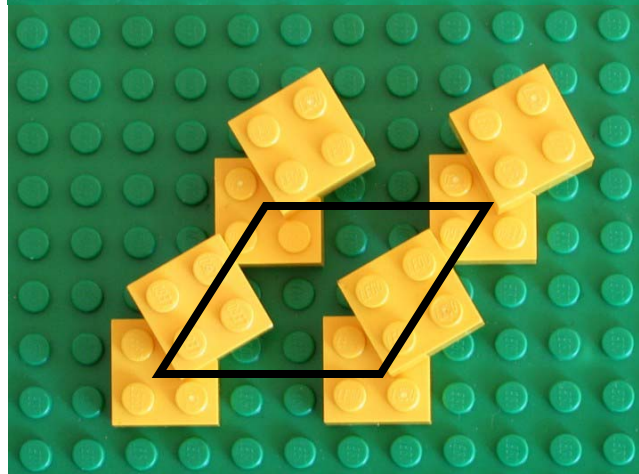


Helix of  
seven  
atoms

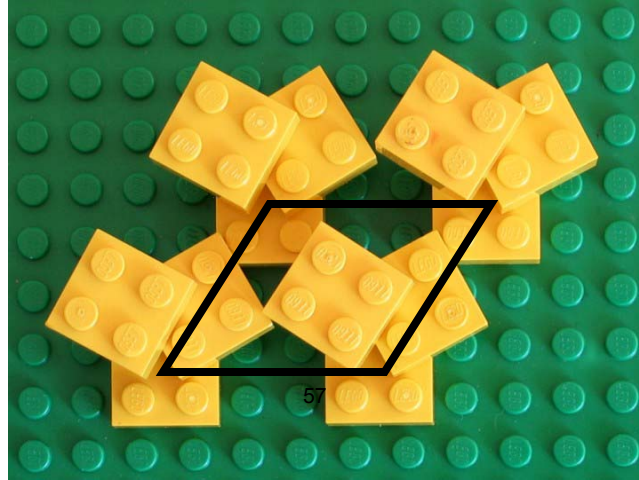
$Z=0,1$



$Z=0.333$



$Z=0.667$





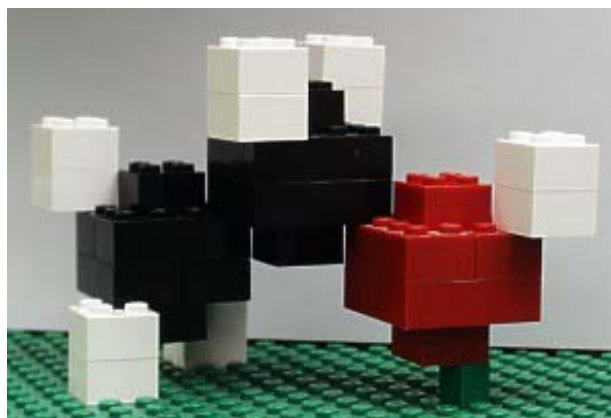
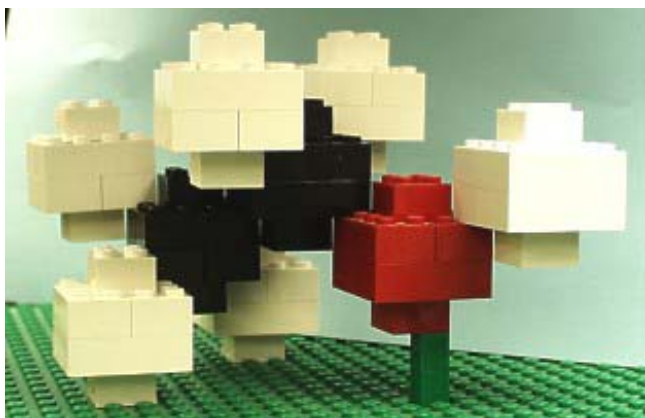
# Organic Compounds



Models of organic compounds can be made from tetrahedral bonded LEGO® bricks.

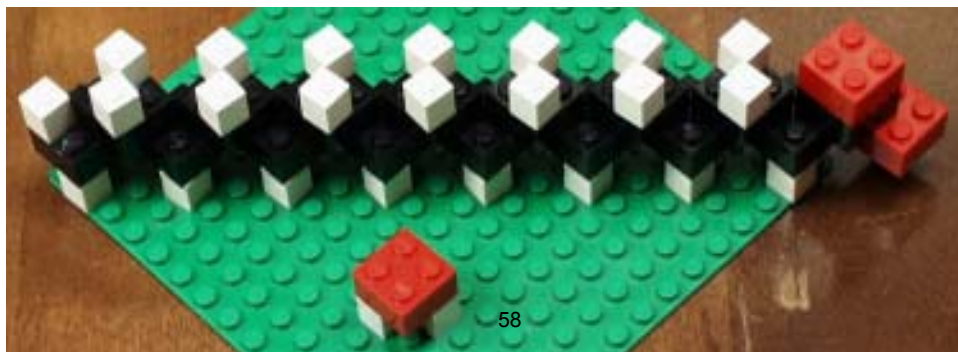
Tetrahedral Bonding

## Ethanol



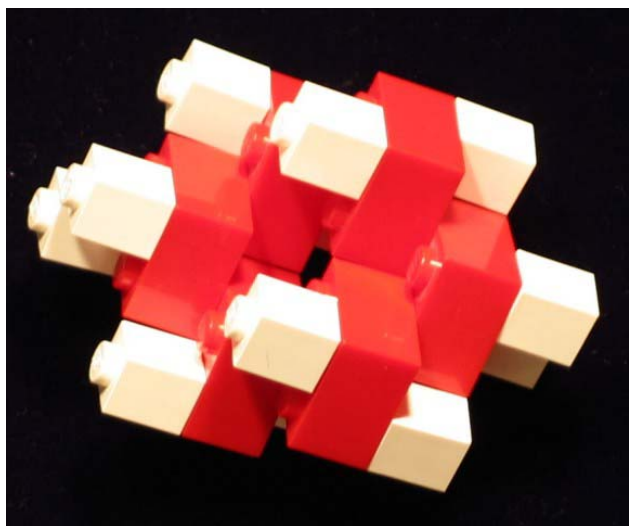
Like many organic chemistry models:  
black = carbon, white = hydrogen, red = oxygen

## Soap (palmitate ion) and Water

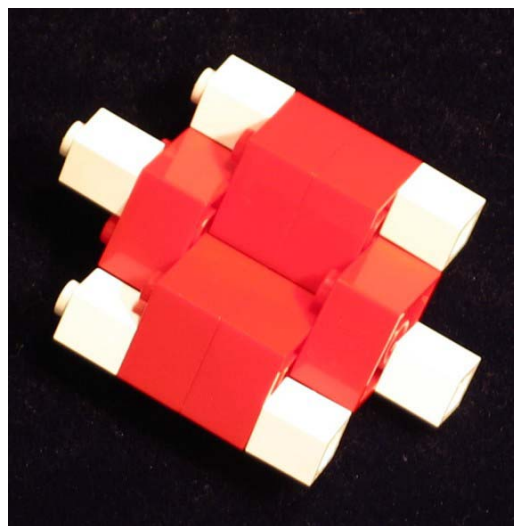


# Organic Compounds

Cyclohexane

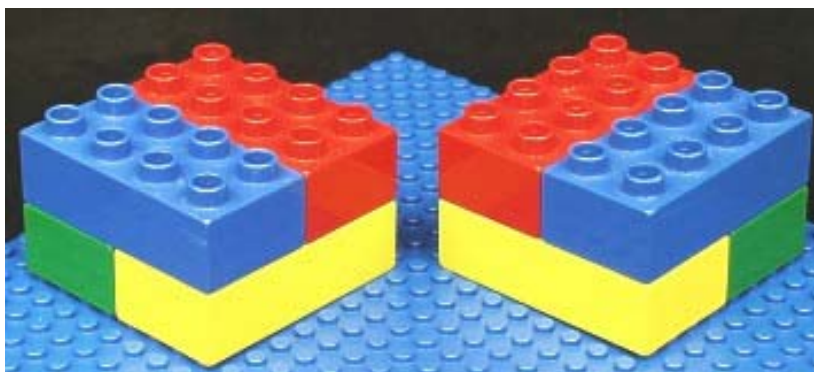


Benzene

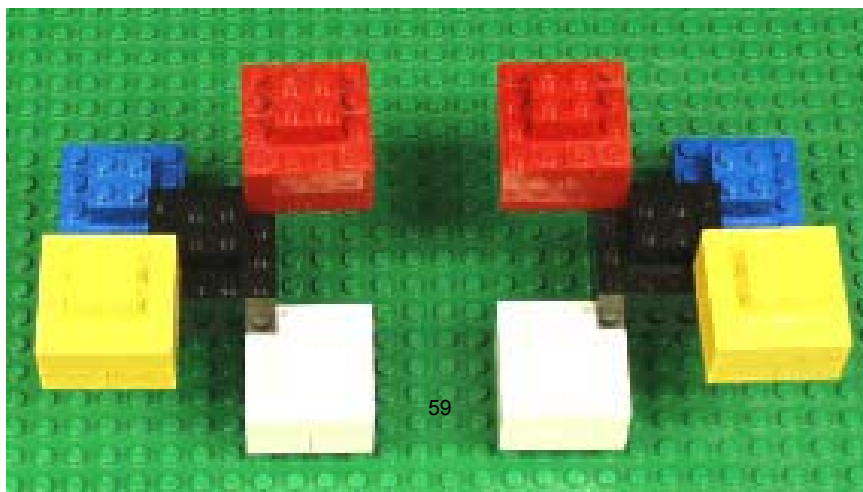


## Chiral Structures

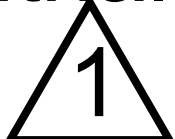
Simplest Structure



Tetrahedral Bonded Structure



# Polyethylene terephthalate

(PET, )

## Color key:

black = carbon

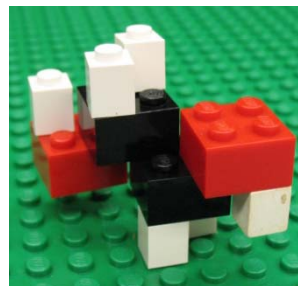
white = hydrogen

red = oxygen

Monomers for the condensation polymerization:

This model requires:

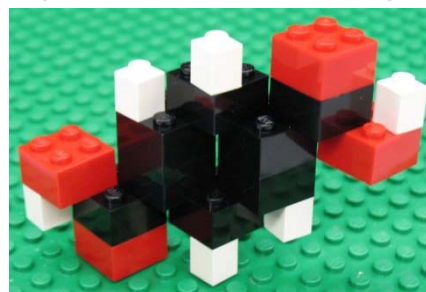
2 red 2x2 bricks  
2 black 2x2 bricks  
6 white 1x1 bricks



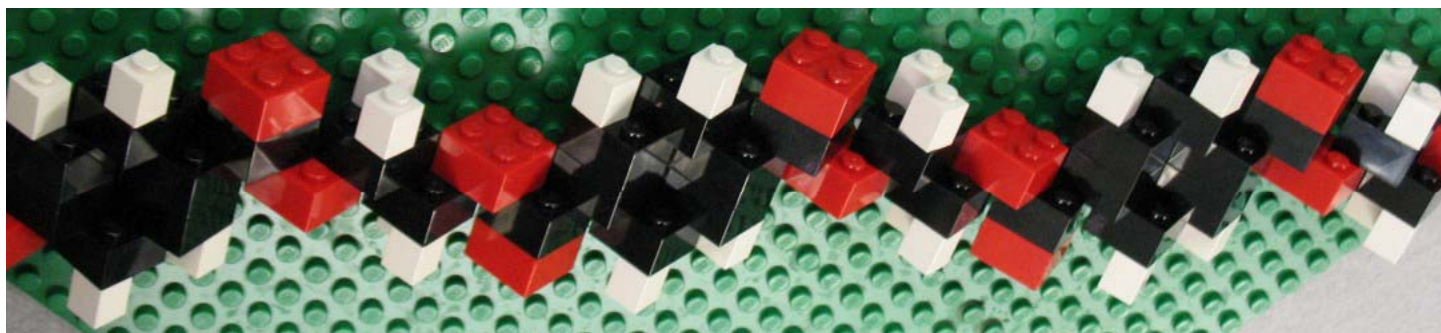
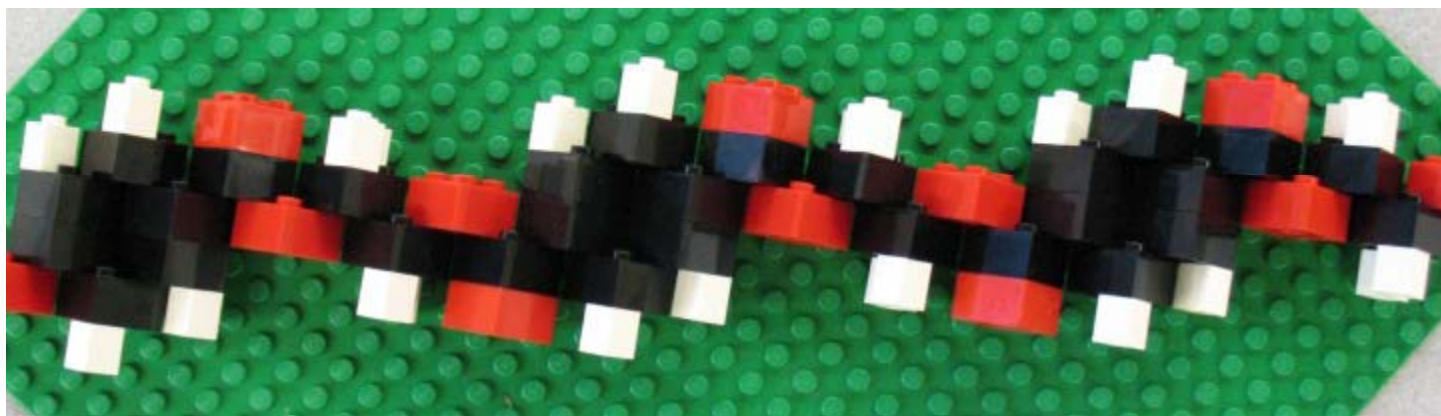
ethylene glycol  
(1,2-ethanediol)

This model requires:

8 black 2x2 bricks  
4 red 2x2 bricks  
6 white 1x1 bricks



terephthalic acid

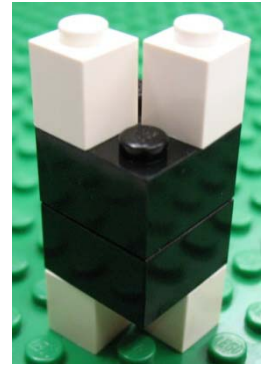




# High Density Polyethylene (HDPE, $\triangle 2$ )

Monomer for the addition polymerization:

This model requires:  
2 black 2x2 bricks  
4 white 1x1 bricks



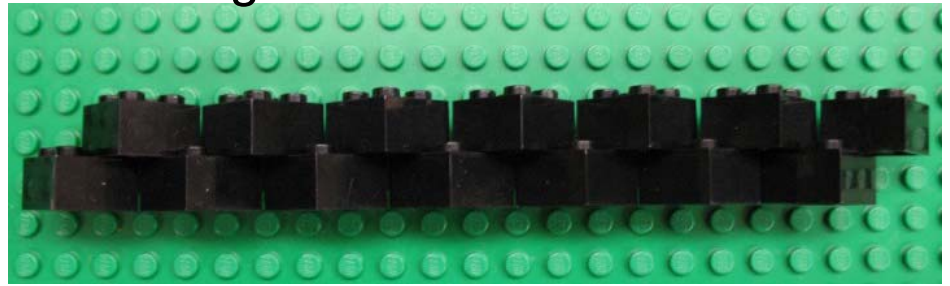
ethylene (ethene)

Color key:

black = carbon

white = hydrogen

Building the carbon backbone first might aid in construction.



The linear polymer chains can pack together closely, causing the polymer to have a higher density than low density polyethylene.



# Polyvinyl chloride

(PVC,  $\triangle_3$ )

## Color key:

black = carbon

white = hydrogen

green = chlorine

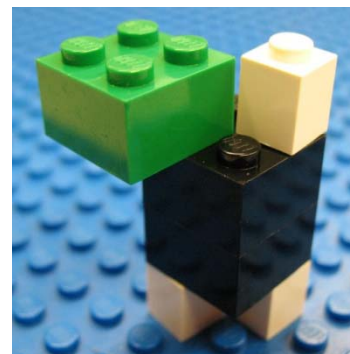
Monomer for  
the addition  
polymerization:

## This model requires:

2 black 2x2 bricks

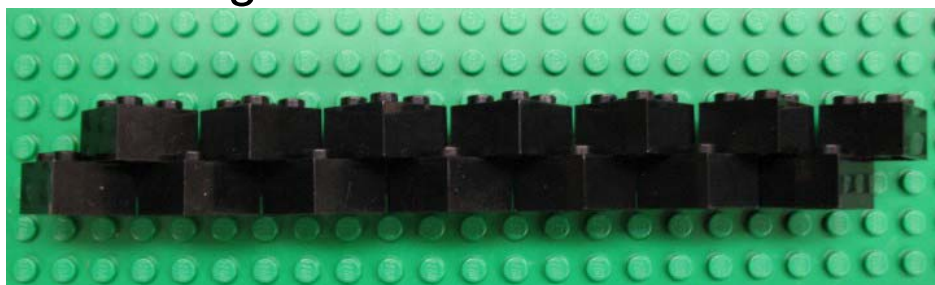
1 green 2x2 brick

3 white 1x1 bricks

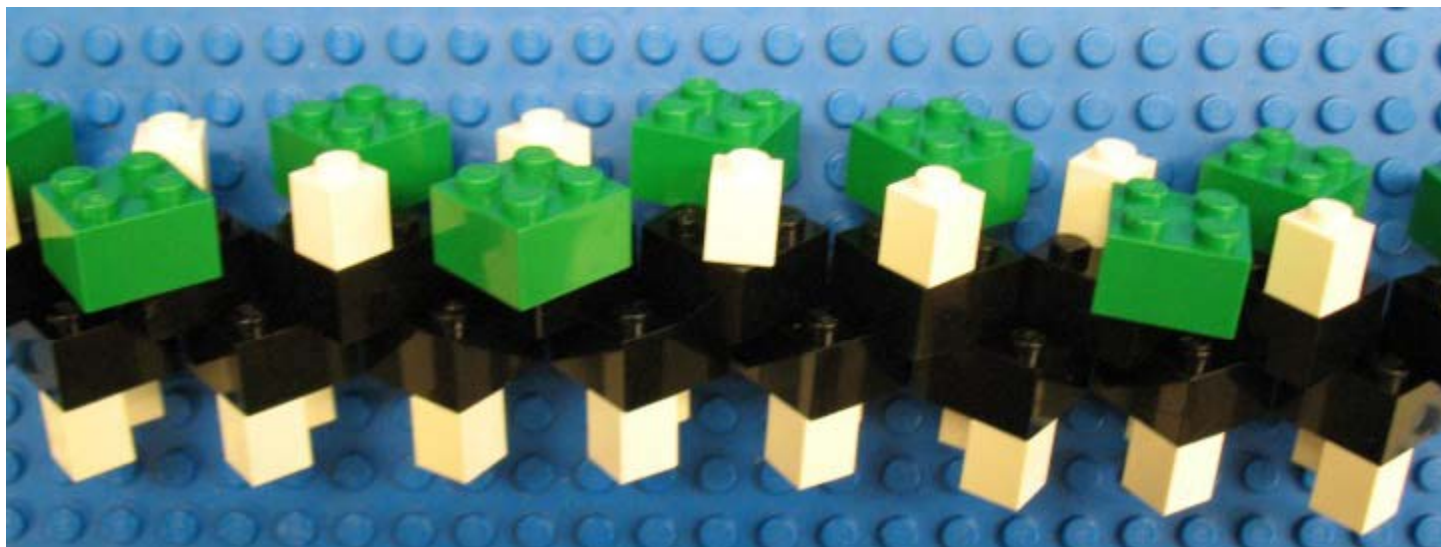


vinyl chloride  
(chloroethene)

Building the carbon backbone first  
might aid in construction.



The structure is very similar to high density polyethylene,  
except one of the two hydrogen atoms on every other  
carbon atom has been replaced with a larger chlorine atom.



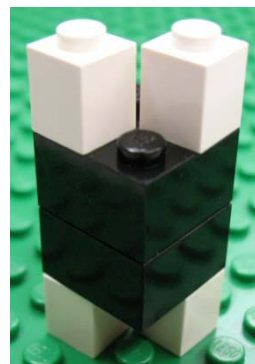
# Low Density Polyethylene (LDPE, $\triangle 4$ )

Monomer for the addition polymerization:

This model requires:

2 black 2x2 bricks

4 white 1x1 bricks



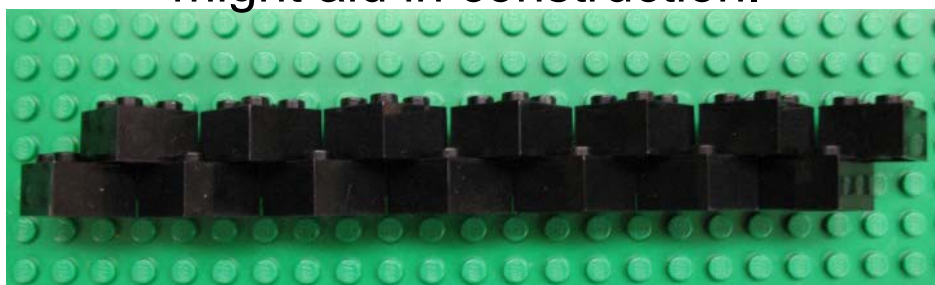
ethylene (ethene)

Color key:

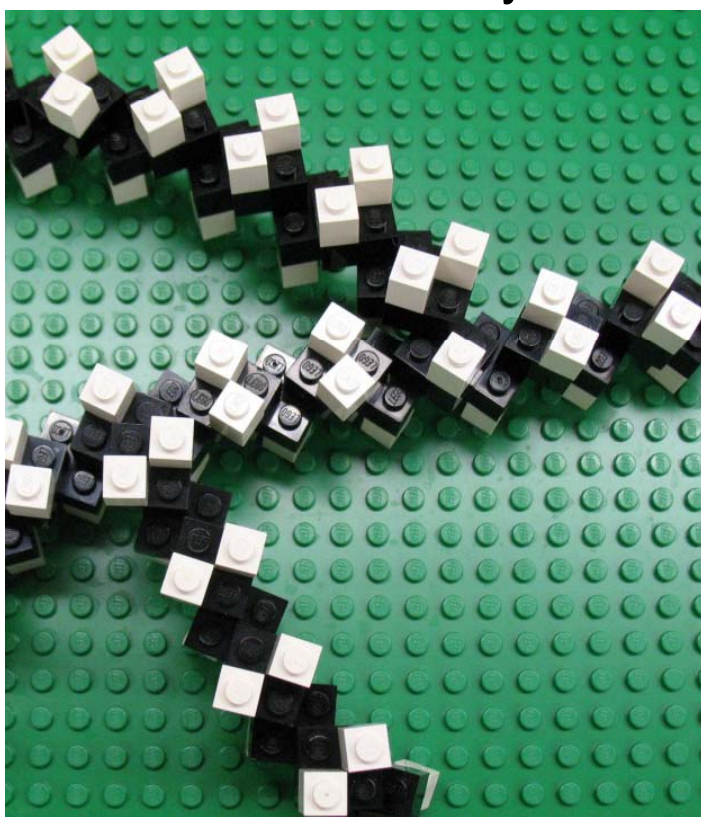
black = carbon

white = hydrogen

Building the carbon backbone first might aid in construction.



The branching polymer chains pack together loosely, causing the polymer to have a lower density than high density polyethylene.





# Polypropylene (PP, $\triangle 5$ )

## Color key:

black = carbon

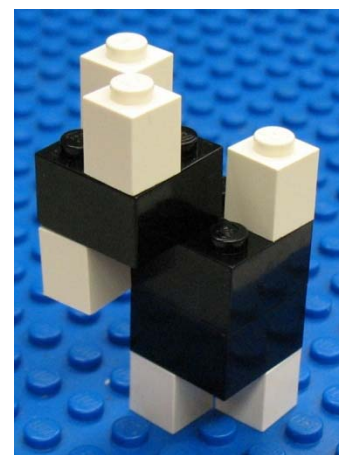
white = hydrogen

Monomer for  
the addition  
polymerization:

This model requires:

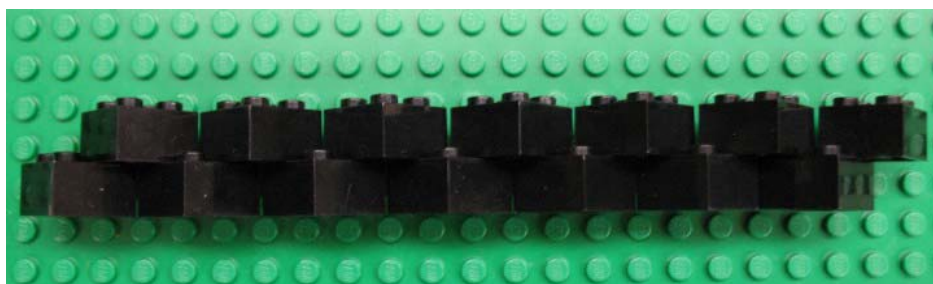
3 black 2x2 bricks

6 white 1x1 bricks

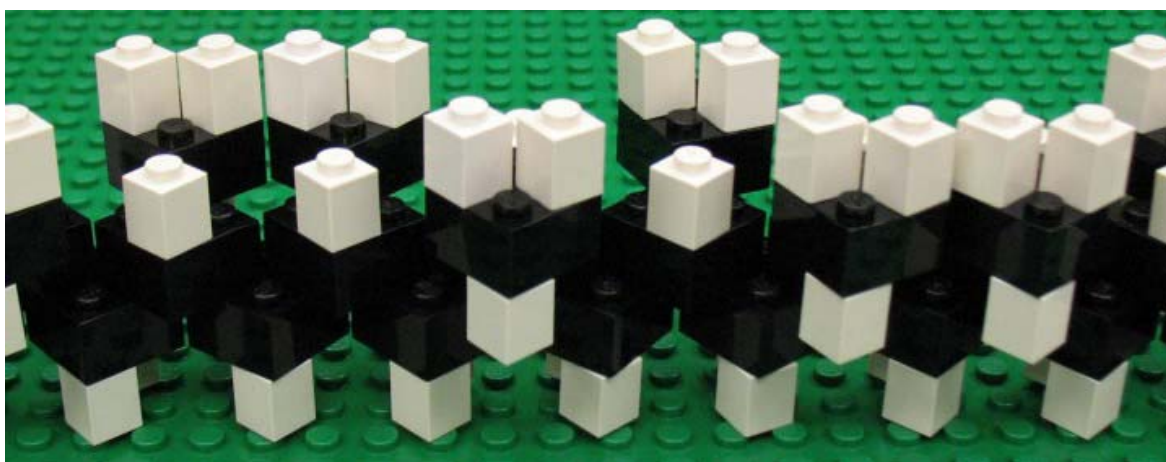
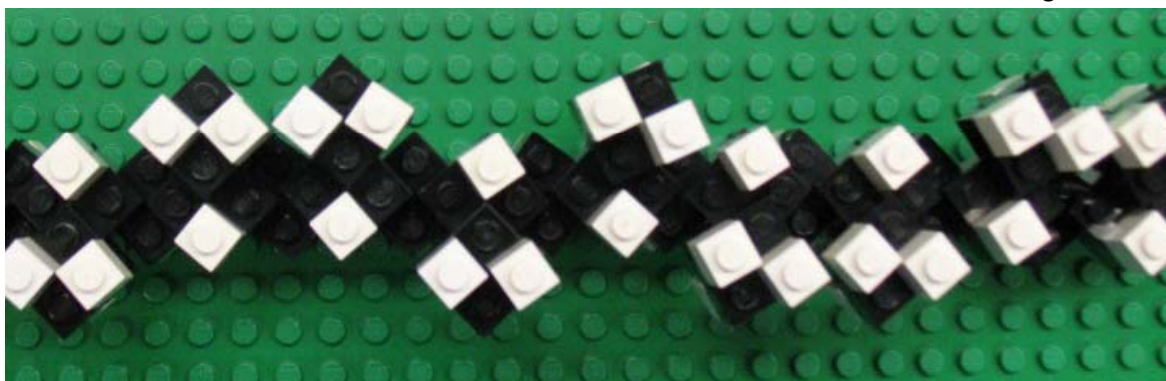


propylene  
(propene)

Building the carbon  
backbone first might  
aid in construction.



The structure is very similar to high density polyethylene,  
except one of the two hydrogen atoms on every other  
carbon atom has been replaced with methyl ( $\text{CH}_3$ ) group.



# Polystyrene (PS, $\triangle_6$ )

## Color key:

black = carbon

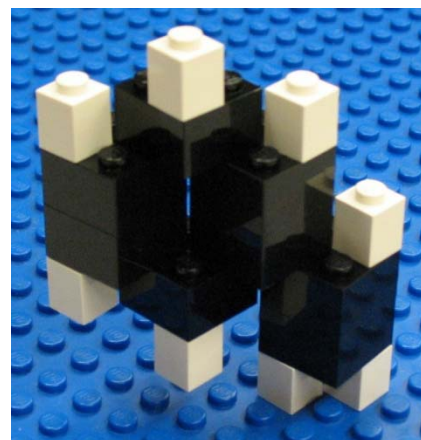
white = hydrogen

Monomer for  
the addition  
polymerization:

This model requires:

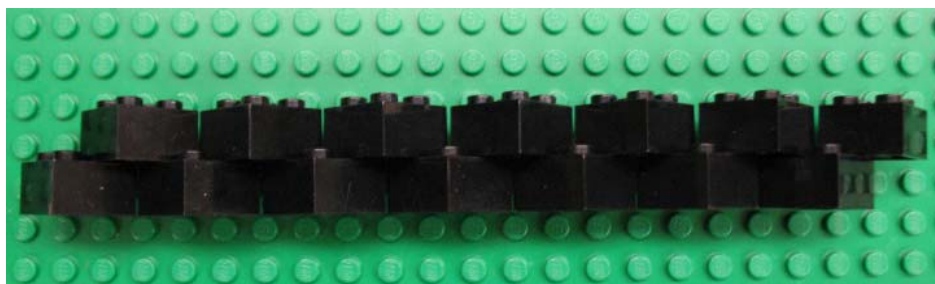
8 black 2x2 bricks

9 white 1x1 bricks

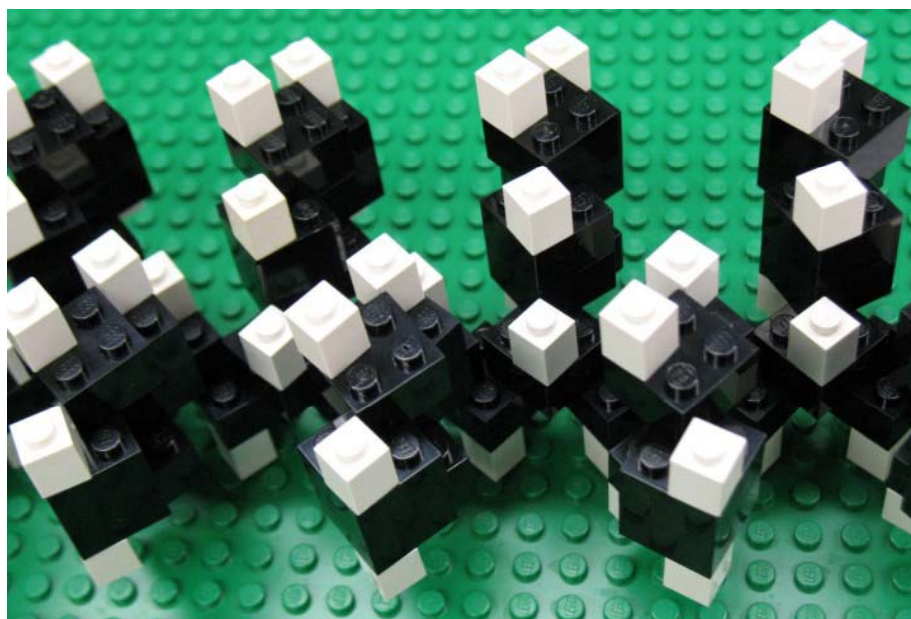


styrene

Building the carbon  
backbone first might  
aid in construction.



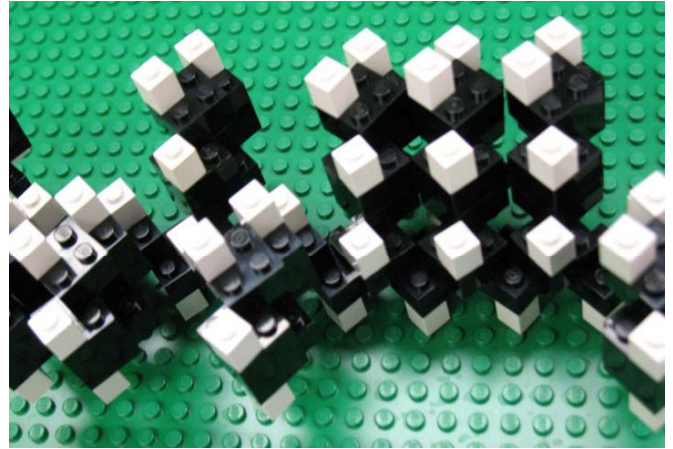
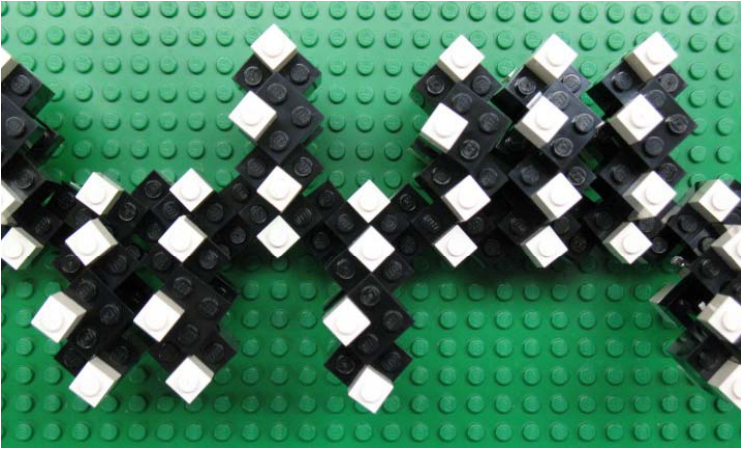
The structure is similar to high density polyethylene, except one of the two hydrogen atoms on every other carbon atom has been replaced with phenyl ( $-\text{C}_6\text{H}_5$ ) group. These bulky groups reduce the flexibility of the chains and produce a relatively stiff polymer.



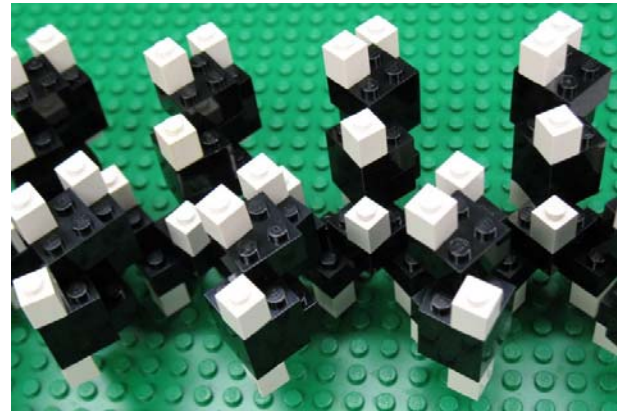
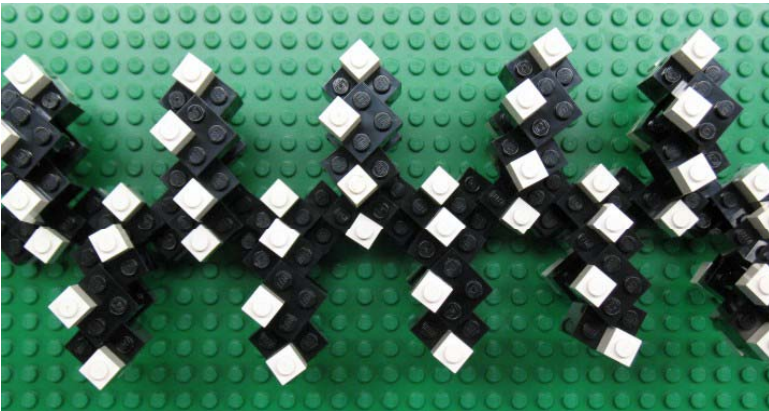


Polystyrene can be produced with varying arrangements of the phenyl groups along their chains.

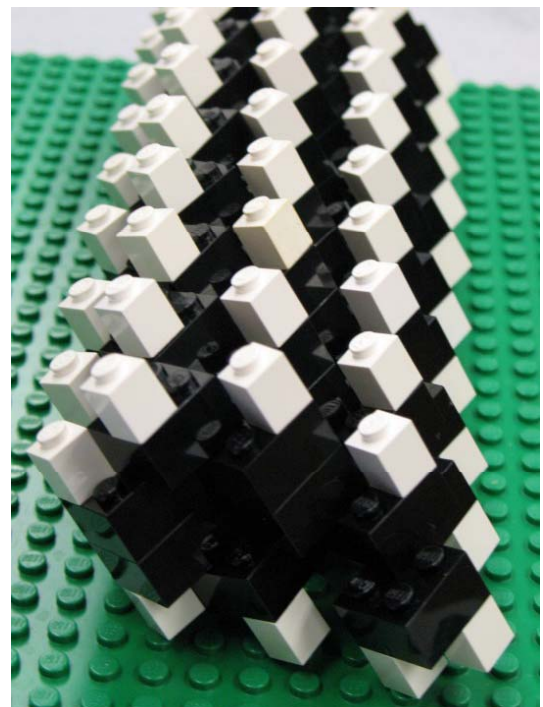
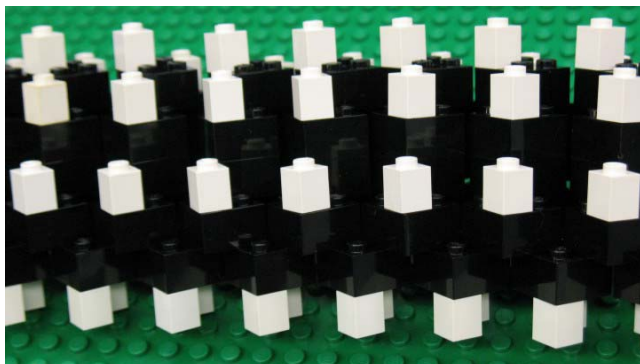
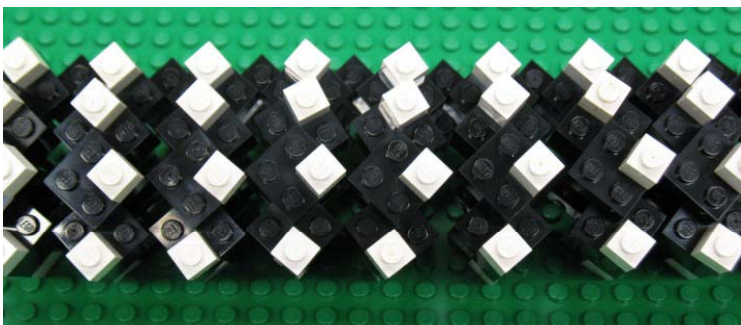
Atactic polystyrene has phenyl groups located randomly on either side of the chain.



Syndiotactic polystyrene has alternating phenyl groups located on opposite sides of the chain.



Isotactic polystyrene has all phenyl groups located on the same side of the chain.



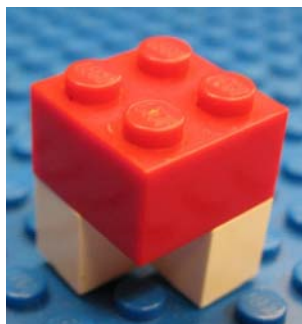


# Polydimethylsiloxane

Monomers for the condensation polymerization:

Color key:

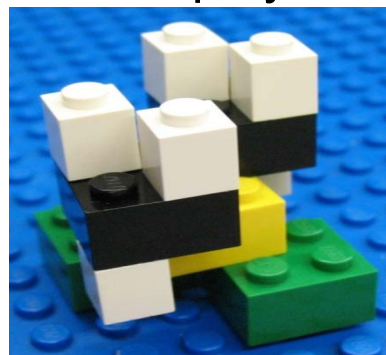
yellow = silicon  
black = carbon  
white = hydrogen  
red = oxygen  
green = chlorine



water

This model requires:

1 red 2x2 brick  
2 white 1x1 bricks

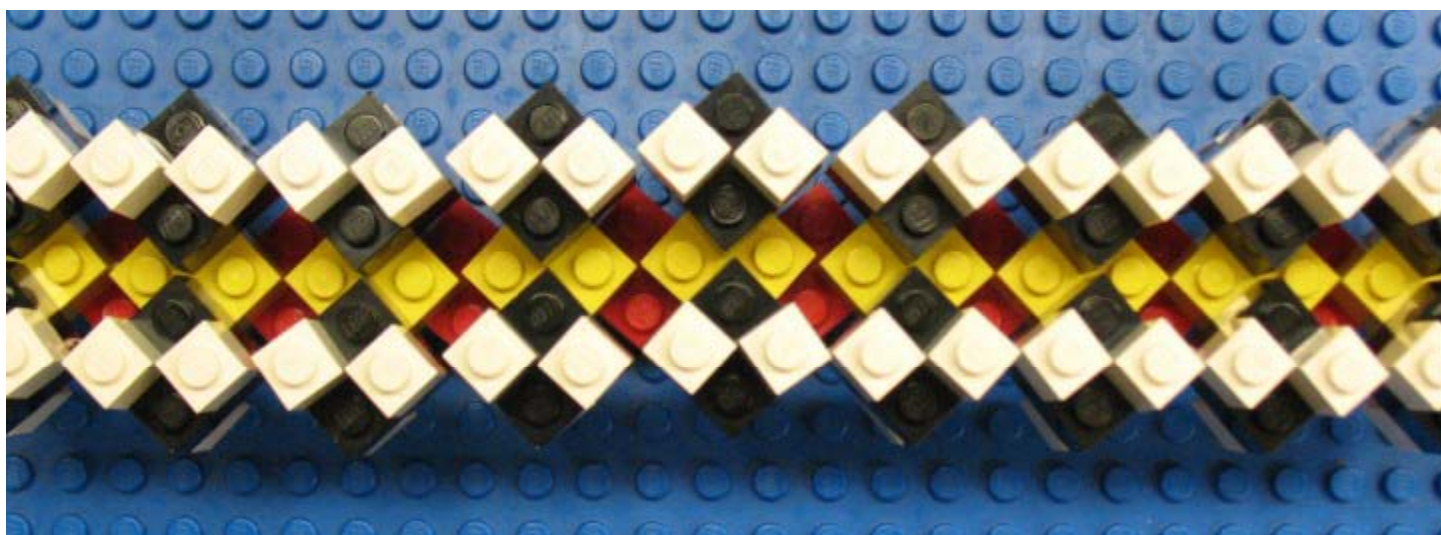


dichlorodimethylsilane

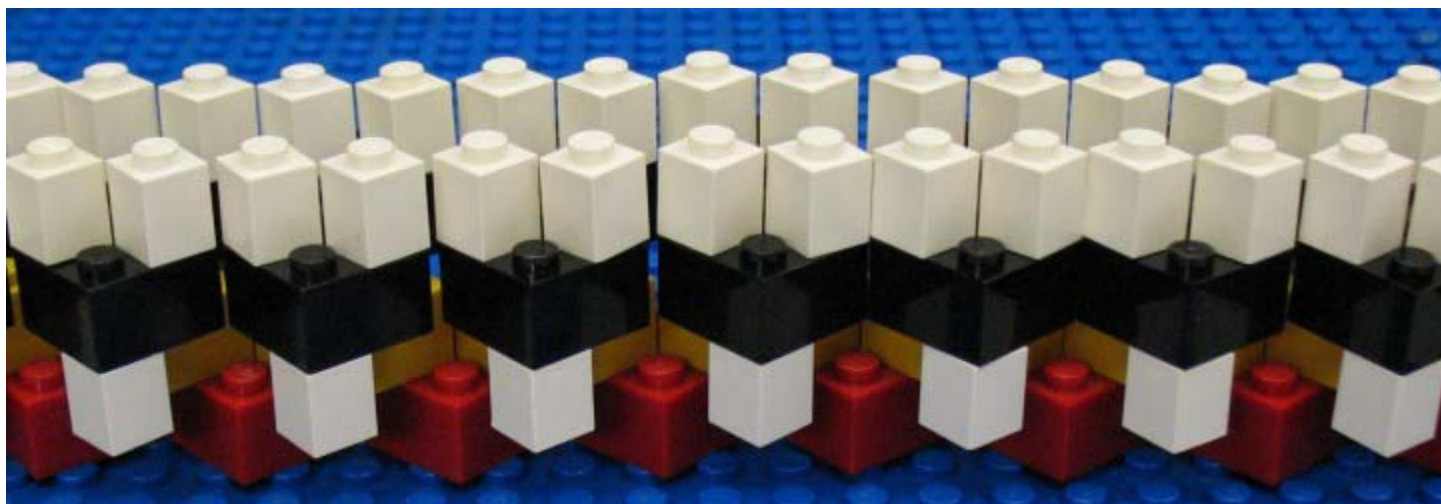
This model requires:

2 green 2x2 bricks  
1 yellow 2x2 brick  
2 black 2x2 bricks  
6 white 1x1 bricks

Top view



Side view

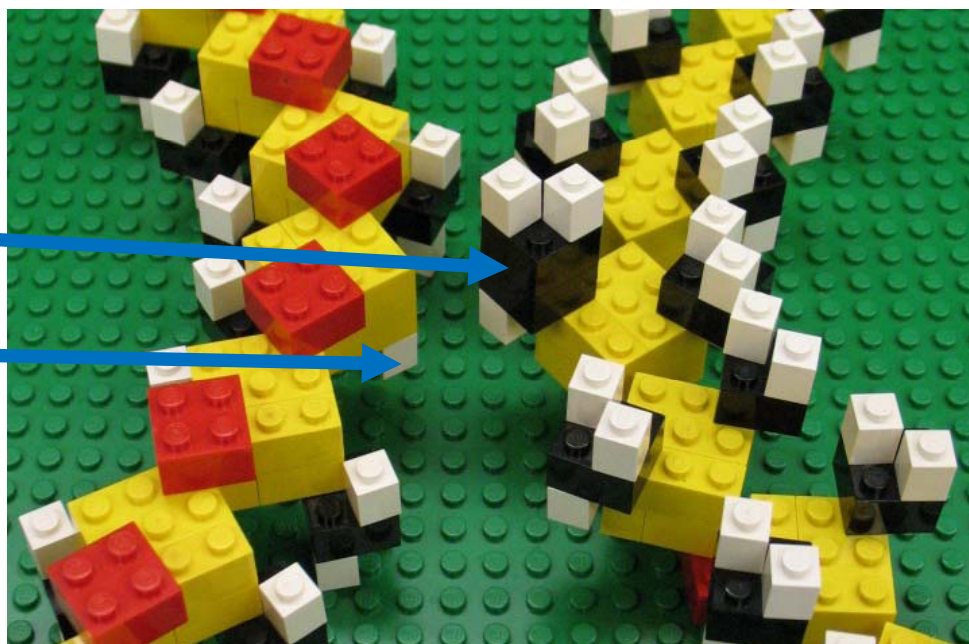




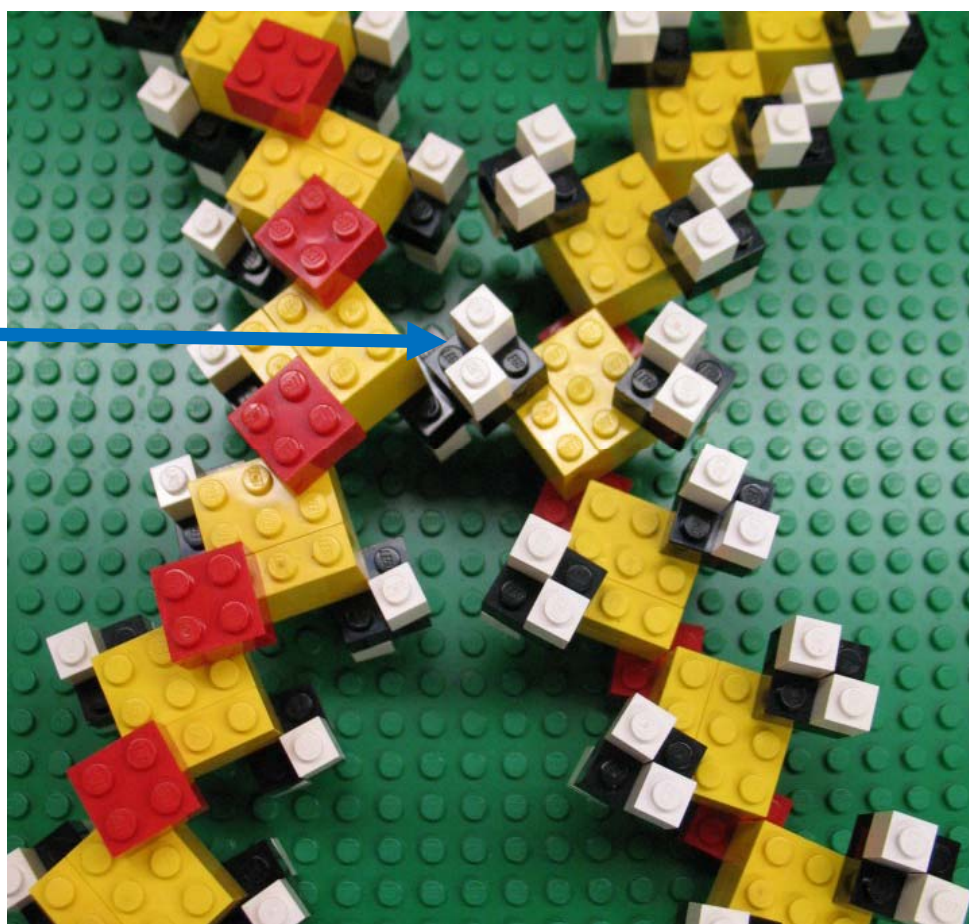
# Polydimethylsiloxane crosslinking via a hydrosilation reaction

The large yellow silicon atoms can be made by placing a 1x3 brick and a 2x3 brick over 1x3 brick and another 2x3 brick.

Before crosslinking, oligomers contain vinyl groups and silane groups. (Note the chains are shown in opposite orientations.)



A hydrosilation reaction crosslinks the oligomers together.



# Nylon-6,6

Monomers for the condensation polymerization:

## Color key:

black = carbon

white = hydrogen

red = oxygen

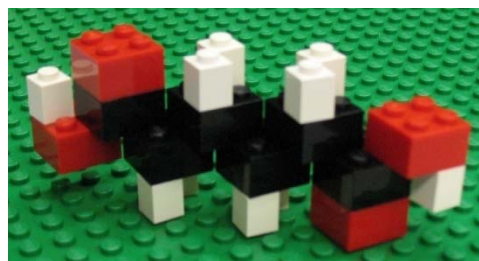
blue = nitrogen

This model requires:

6 black 2x2 bricks

4 red 2x2 bricks

10 white 1x1 bricks



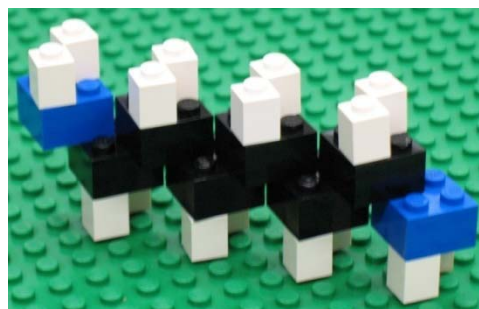
hexanedioic acid

This model requires:

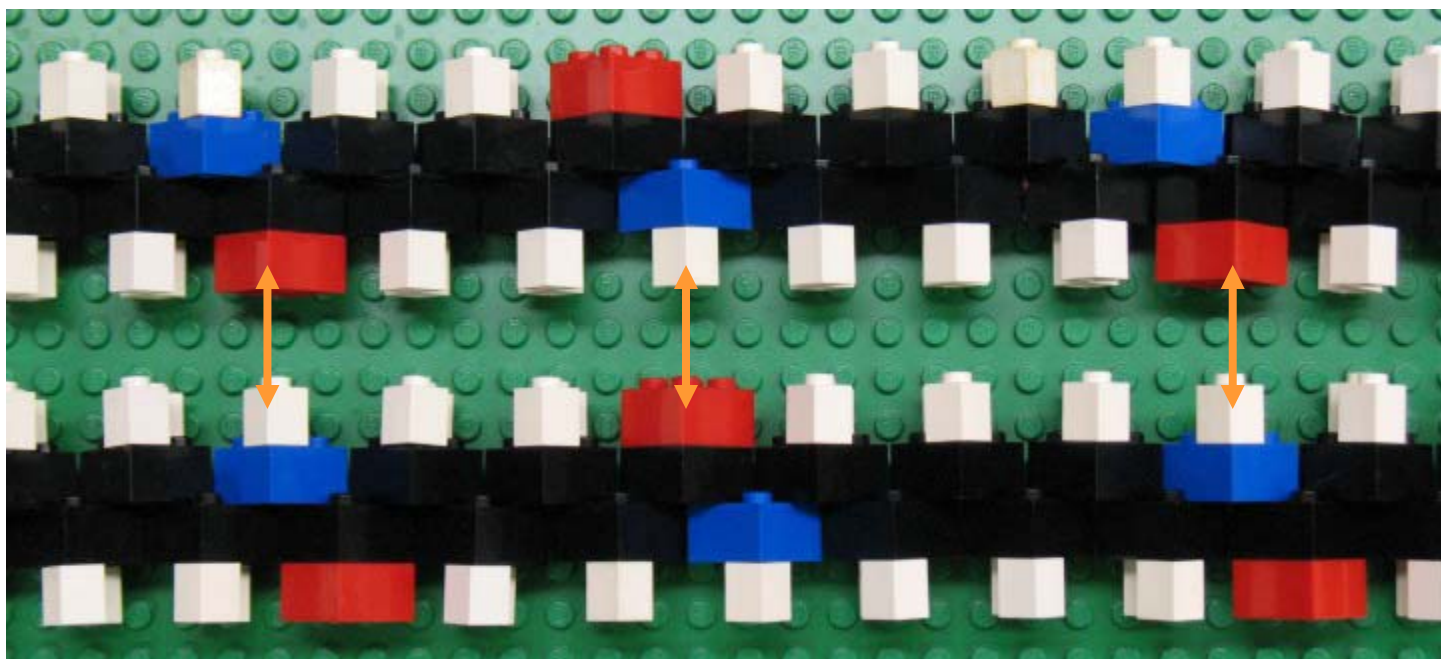
6 black 2x2 bricks

2 blue 2x2 bricks

16 white 1x1 bricks



1,6-diaminohexane



Hydrogen bonding (orange arrows) between oxygen atoms on one polymer strand and hydrogen atoms attached to nitrogen atoms on an adjacent polymer strand help to give nylon its strength.



# Polypeptide (protein)

## Color key:

black = carbon

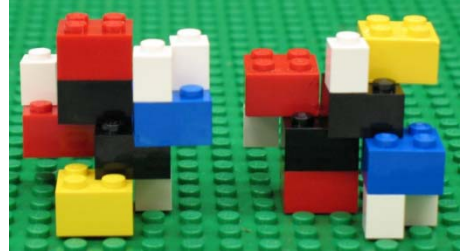
white = hydrogen

red = oxygen

blue = nitrogen

yellow = assorted functional groups

Monomer for the condensation  
polymerization:



amino acid (L isomer)

## This model requires:

35 white 1x1 bricks

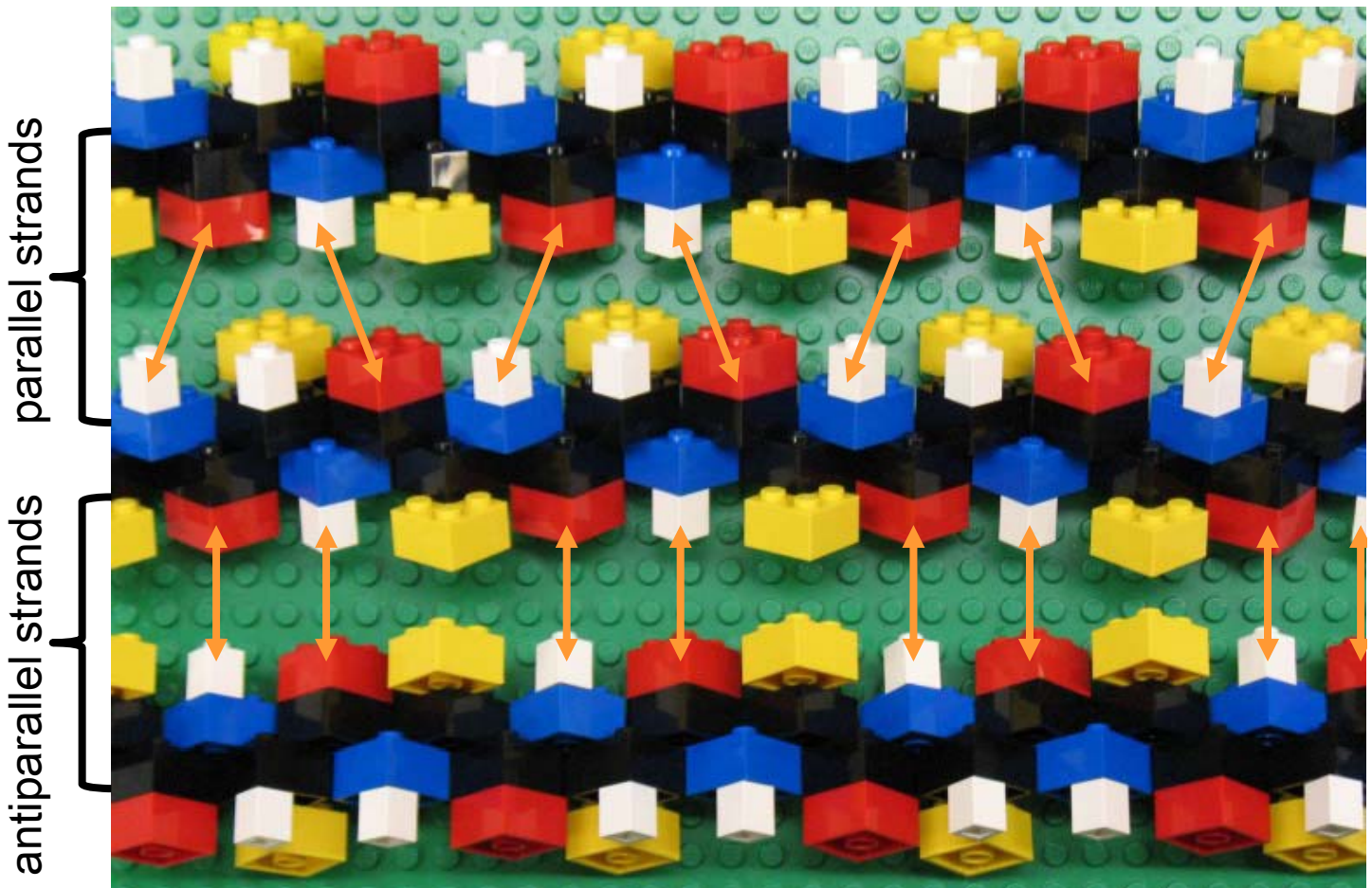
22 red 2x2 bricks

23 blue 2x2 bricks

46 black 2x2 bricks

25 yellow 2x2 bricks

Hydrogen bonds (orange arrows) can form between oxygen atoms on one polymer strand and hydrogen atoms attached to nitrogen atoms on an adjacent polymer strand.



NOTE: Hydrogens connected to the nitrogens on the bottom reversed strand have been moved to the front for ease of viewing.

# Cellulose

*(monomers not shown)*

## Color key:

black = carbon

white = hydrogen

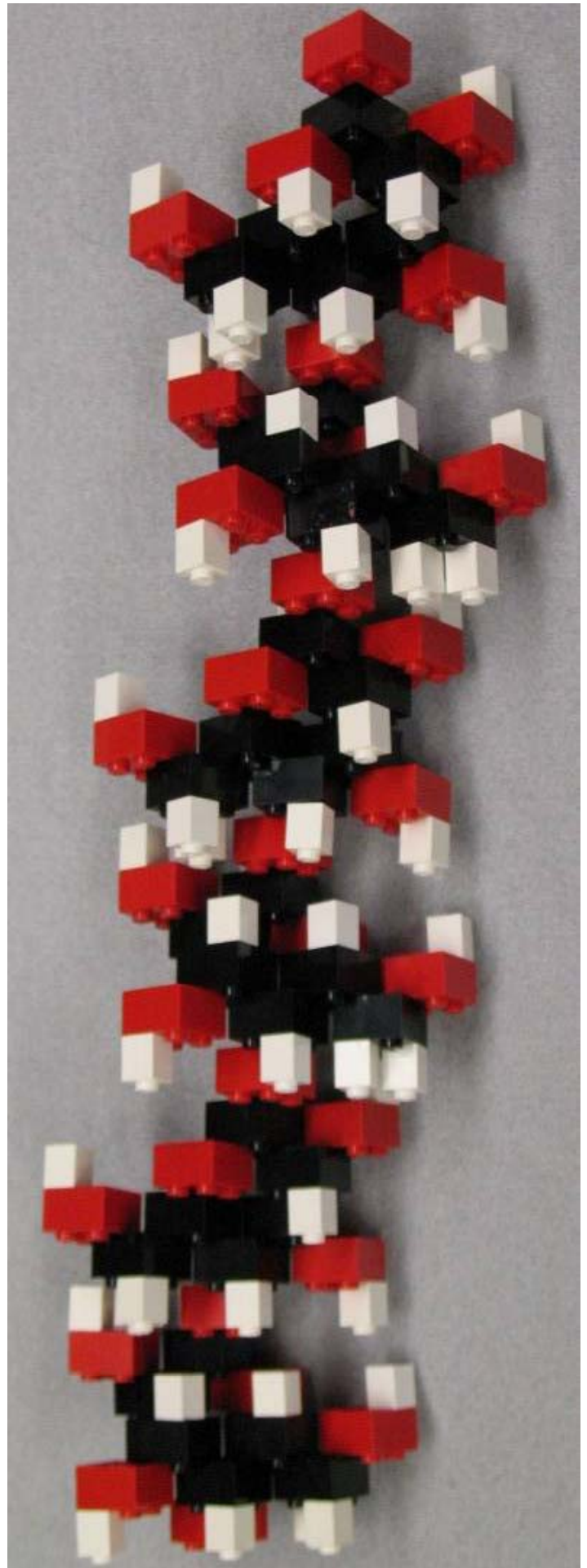
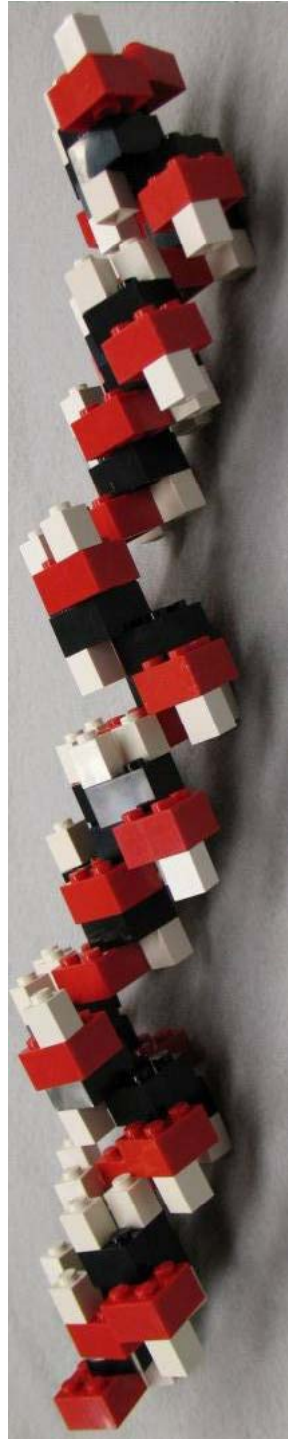
red = oxygen

## This model requires:

34 black 2x2 bricks

31 red 2x2 bricks

45 white 1x1 bricks





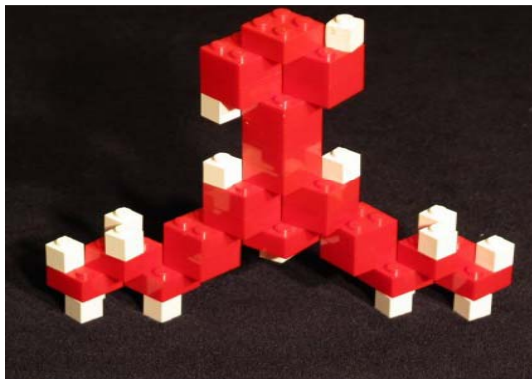
# NanoKid™ Building Steps

NanoKids™ are people-shaped molecules developed at Rice University.

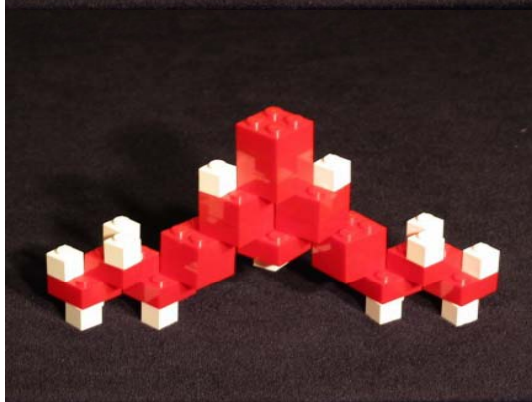
Step

Step

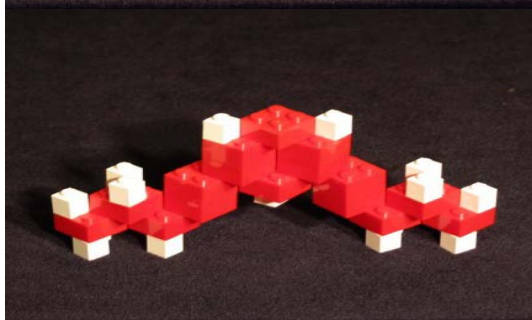
4



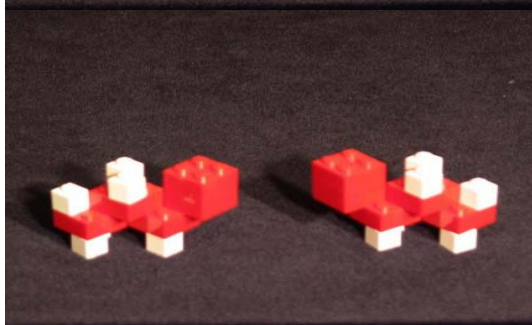
3



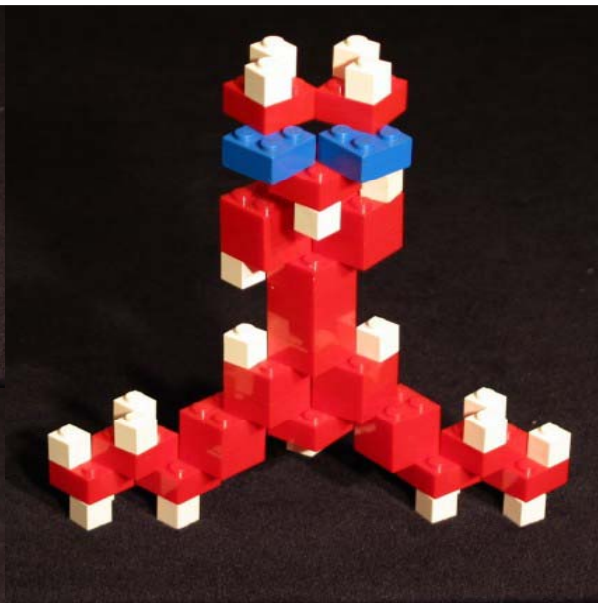
2



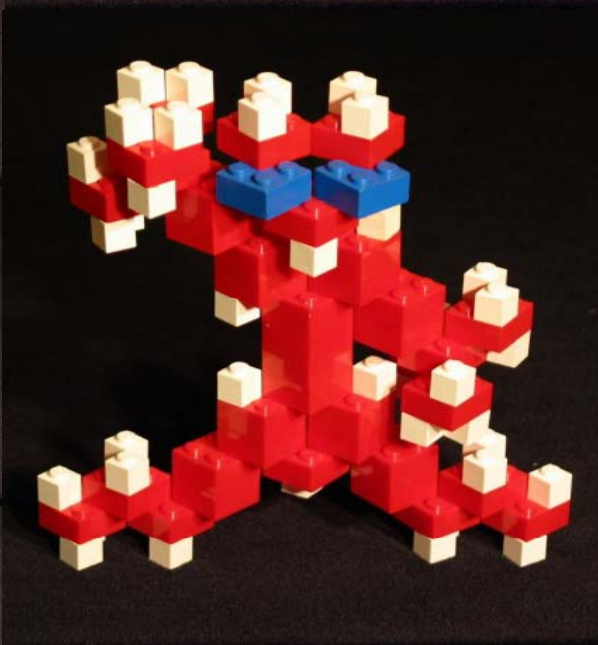
1



5



6



This model requires:

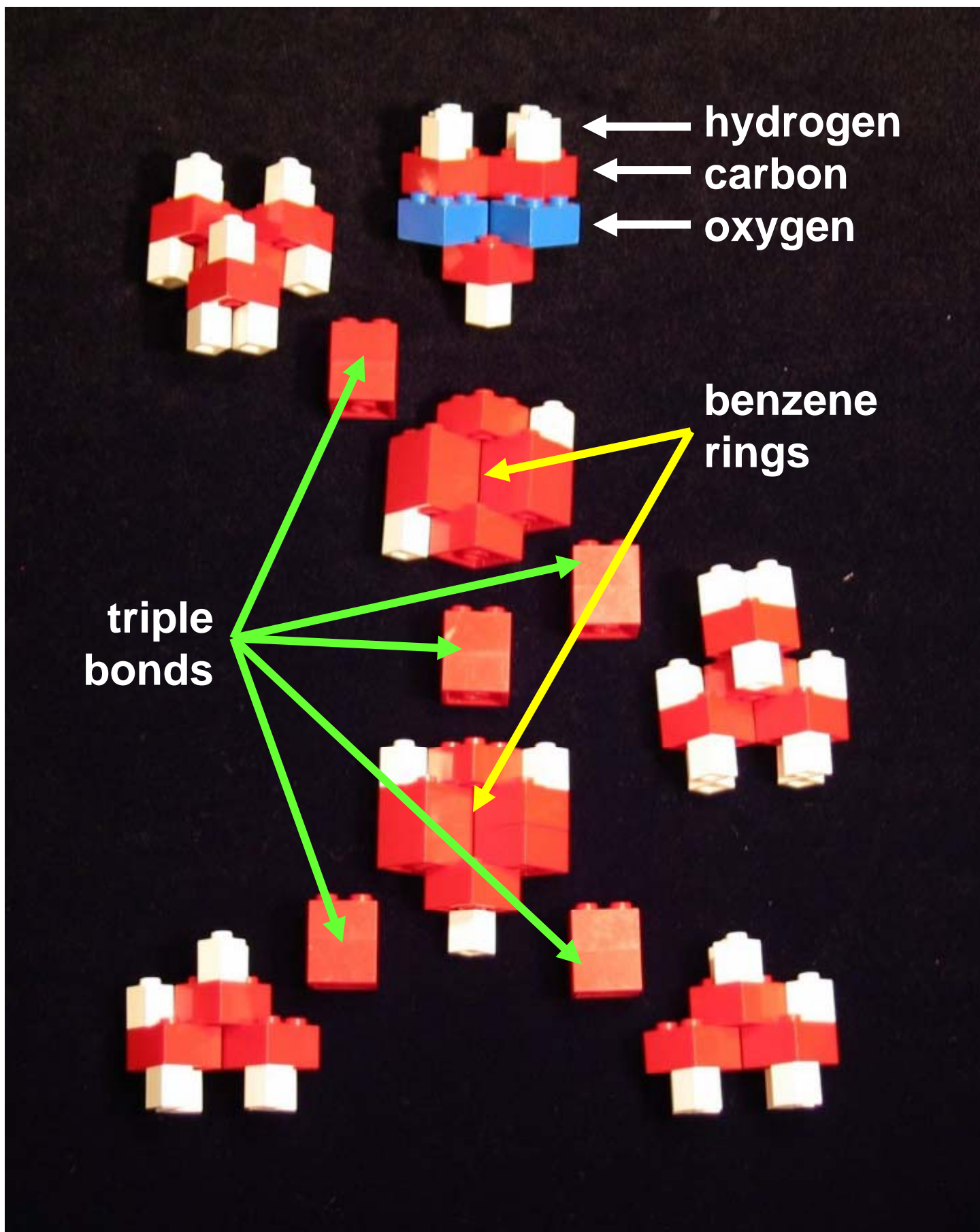
44 white 1x1 bricks

40 red 2x2 bricks

2 blue 2x2 bricks

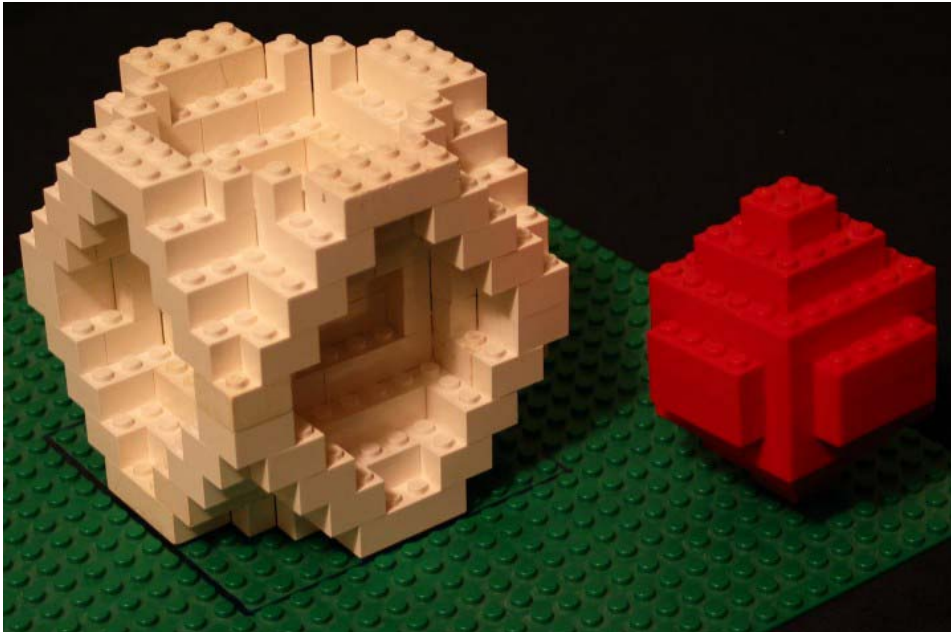


# NanoKid™ Parts



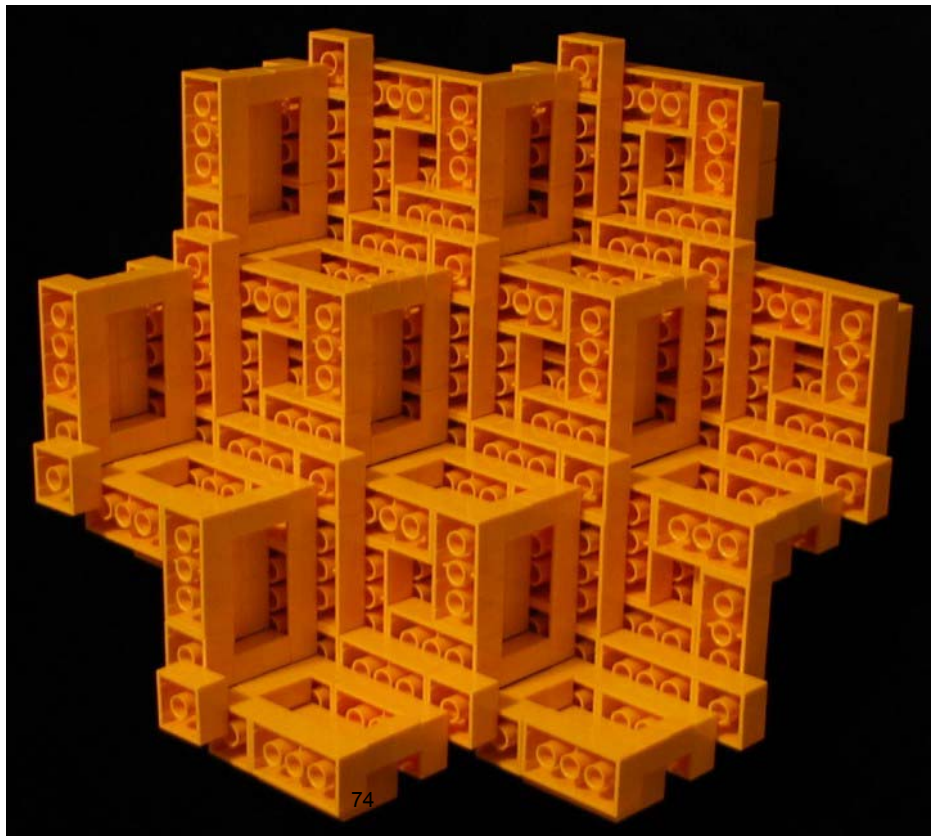
# Face-Centered Cubic Inverse Opal (separated spheres)

Inverse  
opal unit  
cell



Full  
sphere

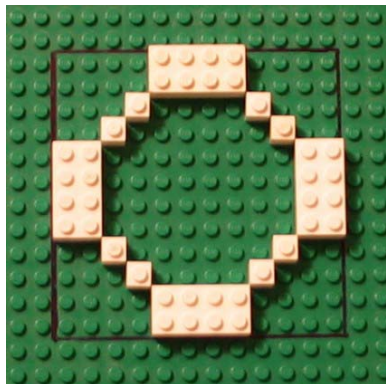
(111)  
interlayer  
structure





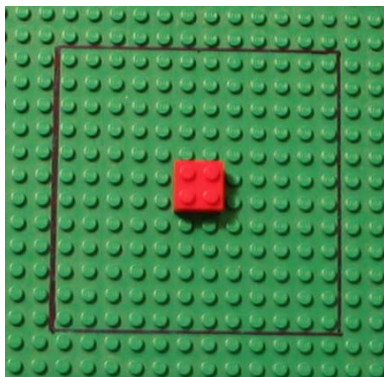
## Opal layers

Layers 1, 10

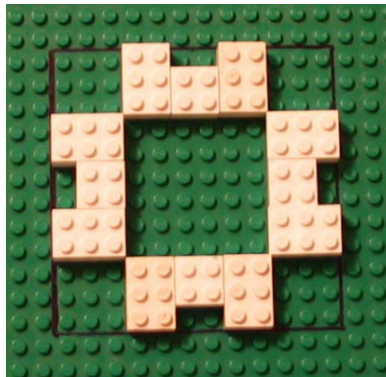


## Sphere layers

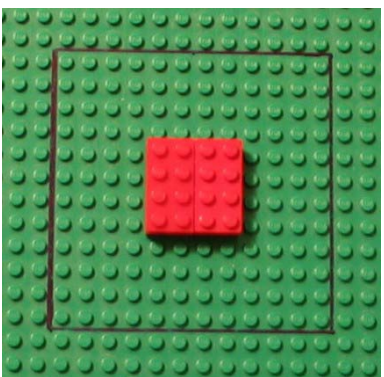
Layers 1, 8



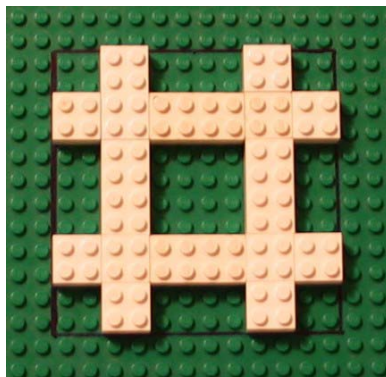
Layer 2, 9



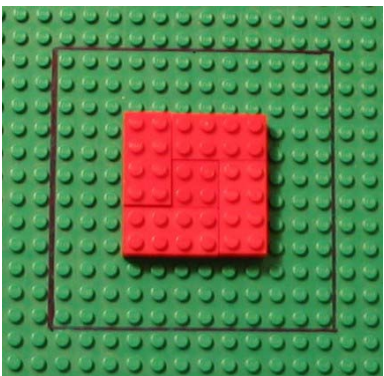
Layers 2, 7



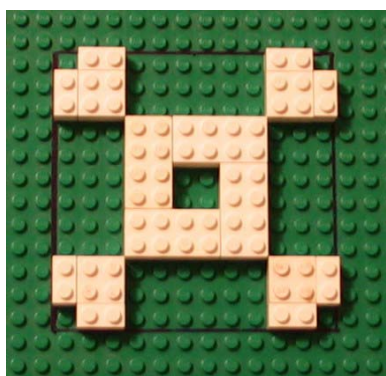
Layer 3, 8



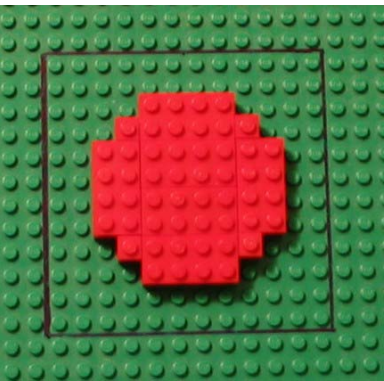
Layers 3, 6



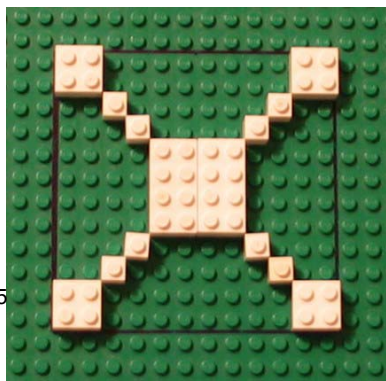
Layer 4, 7



Layers 4, 5



Layer 5, 6



# Face-Centered Cubic Inverse Opal (touching spheres)

Full  
sphere

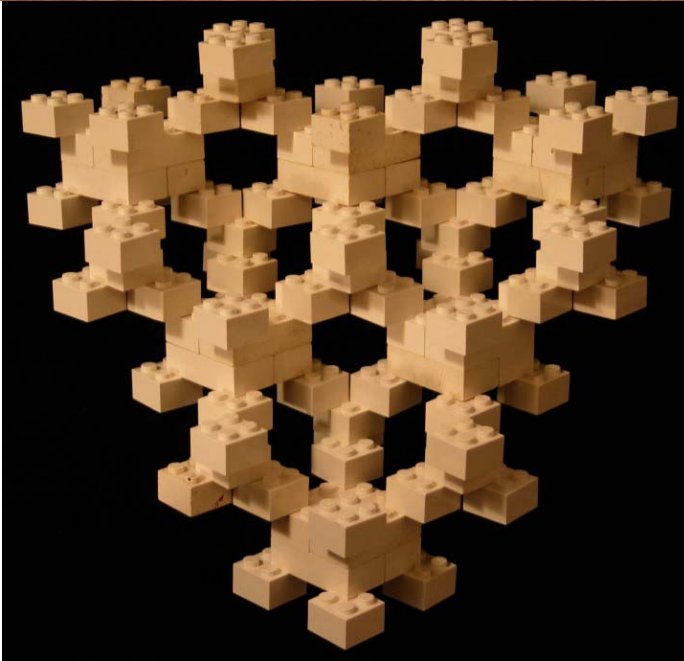
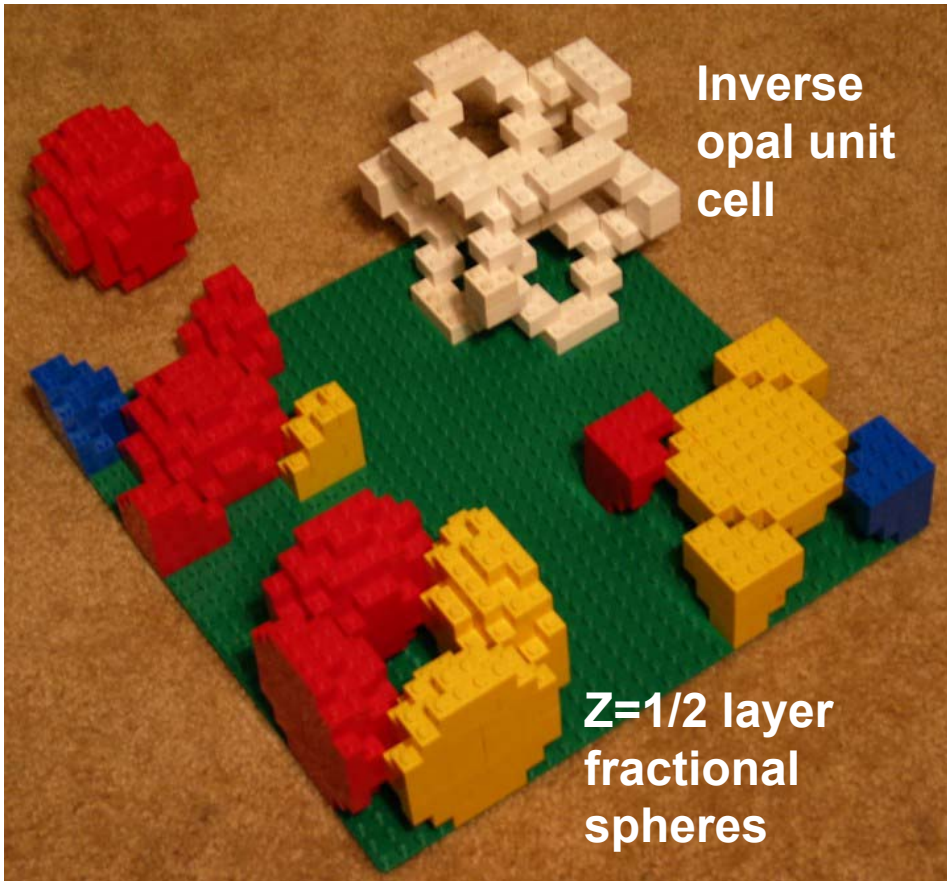
Inverse  
opal unit  
cell

Z=0 layer  
fractional  
spheres

Z=1 layer  
fractional  
spheres

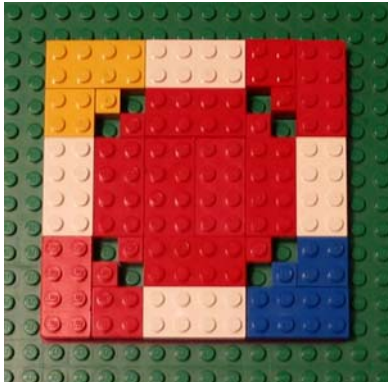
Z=1/2 layer  
fractional  
spheres

(111)  
interlayer  
structure

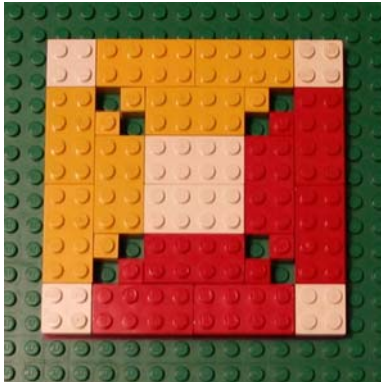




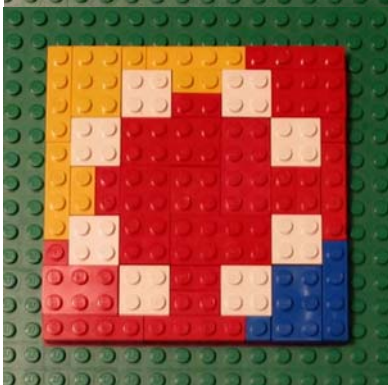
**Layer 1**



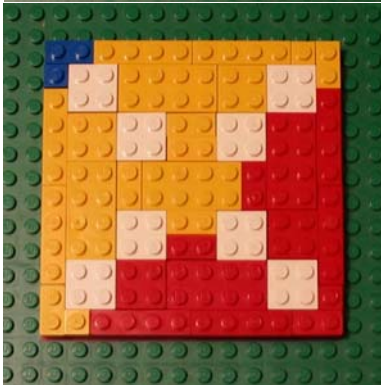
**Layer 6**



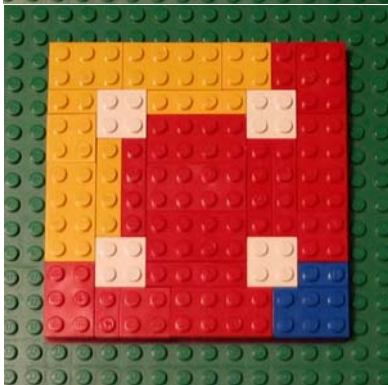
**Layer 2**



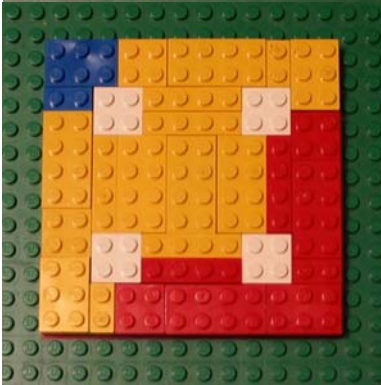
**Layer 7**



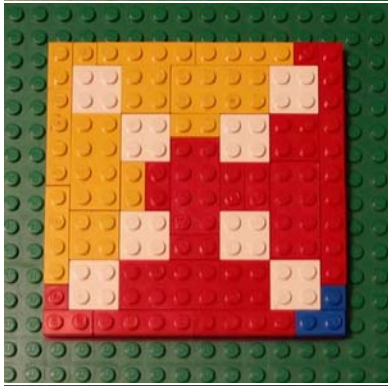
**Layer 3**



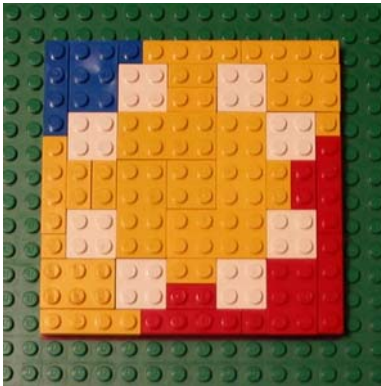
**Layer 8**



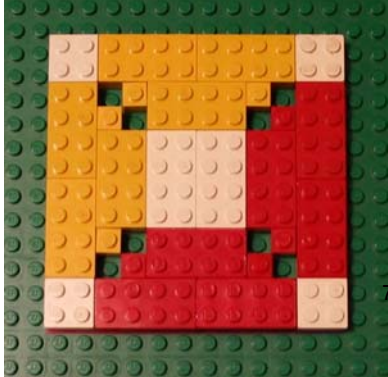
**Layer 4**



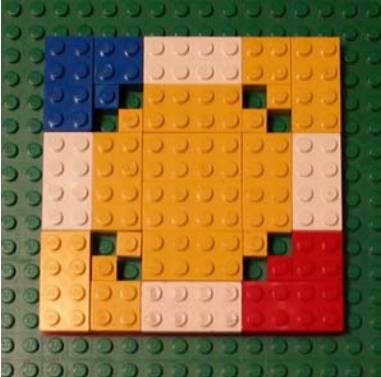
**Layer 9**



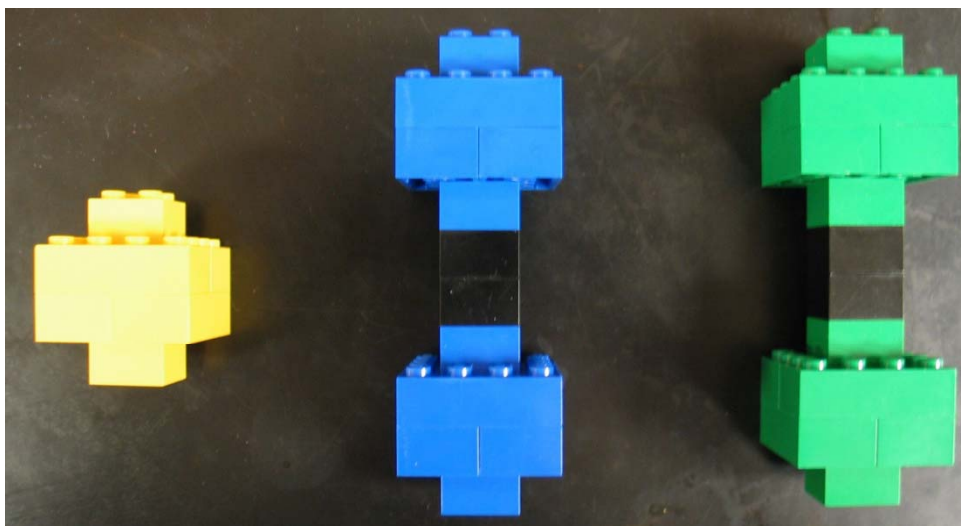
**Layer 5**



**Layer 10**



# Atomic Orbitals



s orbital + p orbital = sp orbital

This model requires:

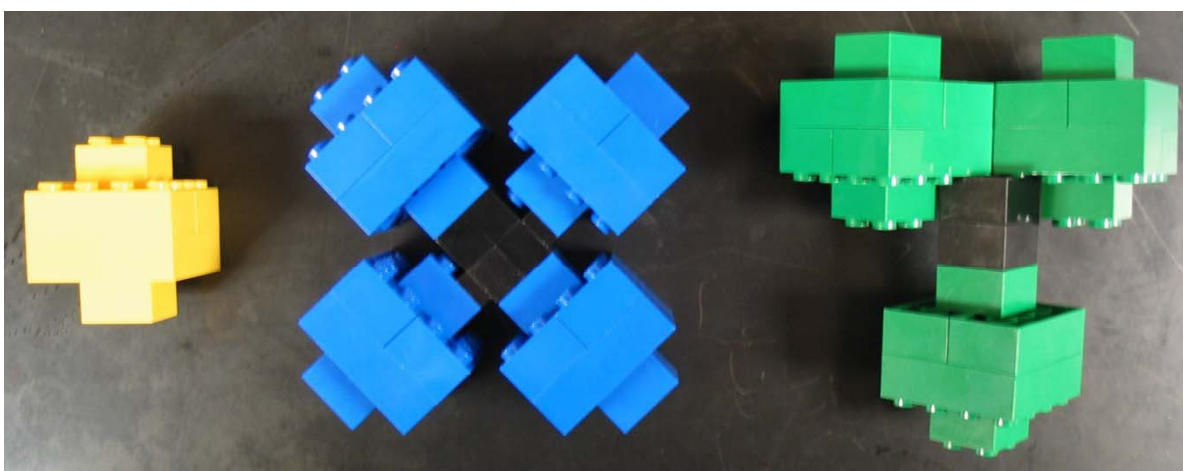
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:

8 blue 2x4 bricks  
4 blue 2x2 bricks  
2 black 2x2 bricks

This model requires:

8 green 2x4 bricks  
4 green 2x2 bricks  
2 black 2x2 bricks



s orbital + two p orbitals = sp<sup>2</sup> orbital

This model requires:

4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:

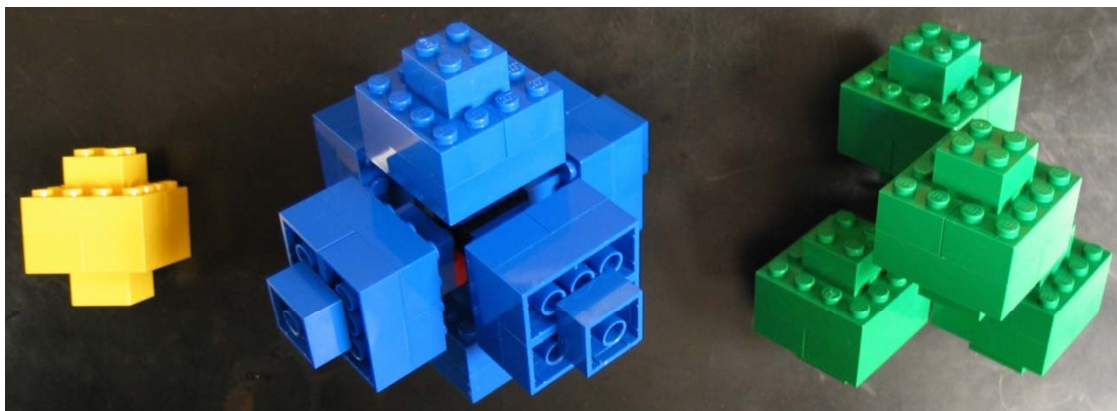
16 blue 2x4 bricks  
8 blue 2x2 bricks  
2 black 2x2 technic bricks  
2 black 1x2 plates w/ 1 knob

This model requires:

12 green 2x4 bricks  
6 green 2x2 bricks  
2 black 2x2 bricks



# Atomic Orbitals



s orbital + three p orbitals =  $sp^3$  orbital

This model requires:

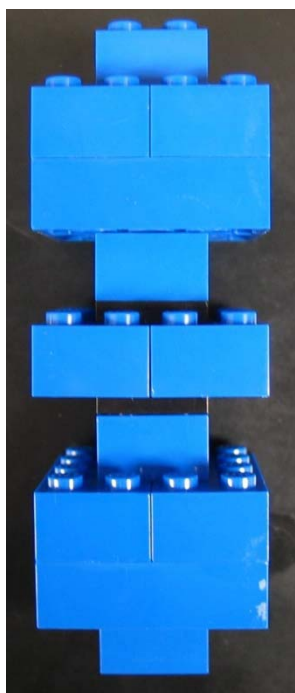
4 yellow 2x4 bricks  
2 yellow 2x2 bricks

This model requires:

24 blue 2x4 bricks  
12 blue 2x2 bricks  
4 black 2x2 technic bricks  
4 black 1x2 plates w/ 1 knob

This model requires:

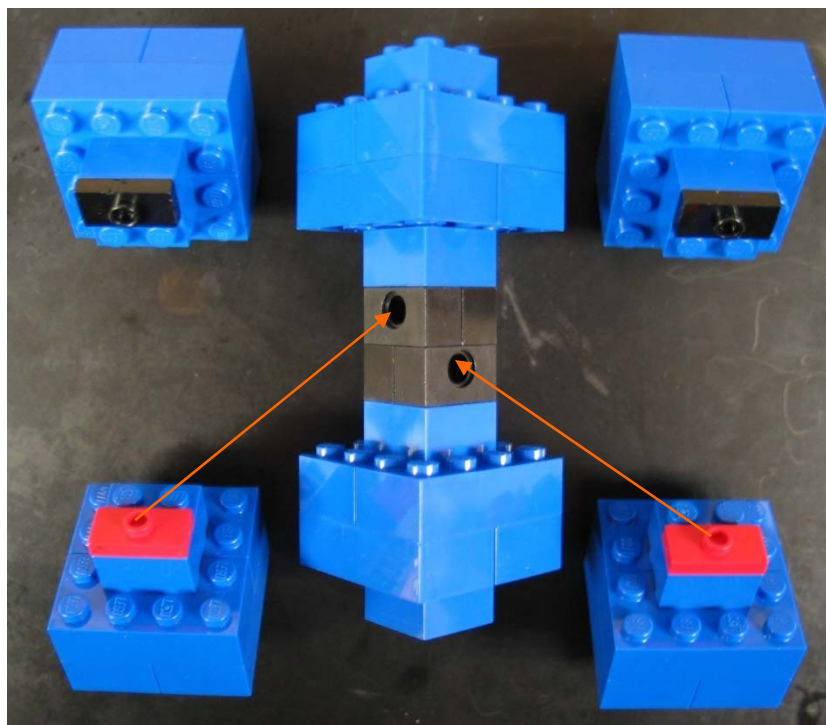
16 green 2x4 bricks  
8 green 2x2 bricks  
2 black 2x2 bricks



$d_{z^2}$  orbital

This model requires:

10 blue 2x4 bricks  
4 blue 2x2 bricks  
2 black 2x2 plates



“three p orbitals” model  
(taken apart for clarity)

same concept used for “two p orbitals” model