MtxGen: A Matrix Generator Library

MtxGen is a built-in option in **PowerMEIS** software package [], which generates matrices for certain shapes and structures of Nanoparticles (NPs).

This guide shows how to generate certain NP shapes and their piling structures.

1) Motivation

Usually, in order to investigate the structural properties of NPs, it is mandatory that these nanoparticles be deposited on a specific substrat. Because of that, it is very common that these NPs agglomerate on the substrate. This agglomeration hardens the study of these NPs, because it hides the real information that comes from idealized NPs monolayers. In order to investigate this agglomeration and its effects in the MEIS spectra, MtxGen library has been developed. In this library, there is a large variety of NPs shape and piling structures. In the following, it will be addressed how to construct such matrices to study NPs.

1) Possible NPs shapes:

Here it is shown all the shapes that can be used in order to generate a NP by the MtxGen matrix generator.

1.1) Spherical NPs

Fig. 1 show the NPs shape that MtxGen can generate.
The following parameters must be specified in the .cpm file in order to generate these structures:

radiusc (core radius) =;
radiusc (shell thickness)=;
radiusc (overall radius, including TOPO)=;

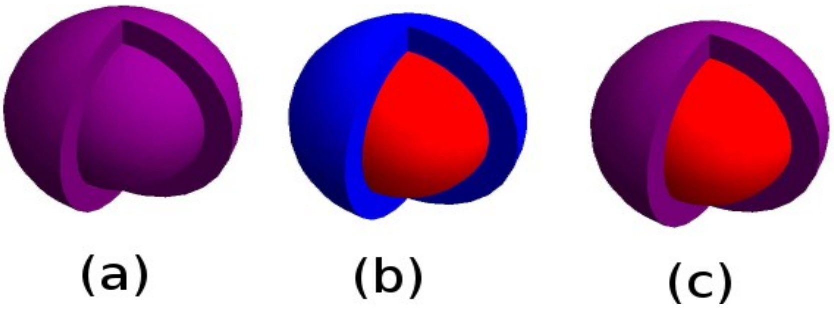


Fig. 1. Three possible NPs structure: (a) a PtPd alloy, (b) Pt@Pd and (c) Pt@PtPd.

1.2) Interpenetrated Spheres NP

Fig. 2 shows this NP shape. It is considered that two NPs overlap, forming an interpenetrated NP. In this overlaping region, as shown in Fig. 2, there is a formation of an alloy composed of both elements (the purple one), possessing a stoichiometry in such a way that the desired stoichiometry is conserved.
In order to generate such a matrix, the following parameters must be specified: (i) first-element radius, (ii) second-element radius, and (iii) the distance between the centers of the NPs.

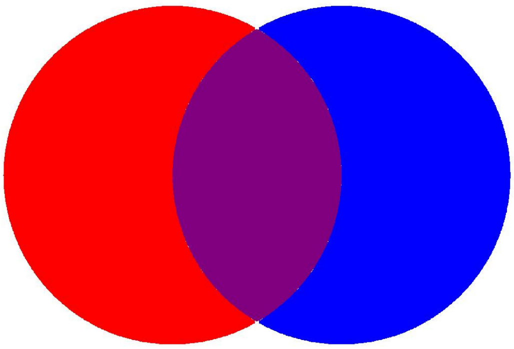


Fig. 2. It shows the typical configuration of two interpenetrated NPs. In the overlaping region (the purple ones), there is an alloy formation. The paramerters to be specified are: (i) first-element radius, (ii) second-element radius, and (iii) the distance between the centers of the NPs.

1.2) Separate Spheres

Here a matrix composed of two elements with a specfic radius are generated by specifying the distance between them. It is noteworthy that these elements can not interpenetrate, but they must be apart from each other. In this configuration, it is necessary to specify the radius of one of these elements, as well as the global stoichiometry to be conversed, and the distance between these NPs. Keeping this in mind, the radius of the second element is obtained straightforwardly.

The distance between the NPs does not affect the calculations.

For this shape, the same configuration of the interpenetraated spheres can be applied, however, with the distance between the spheres must be set as the sum of the radius of the first and second particle.

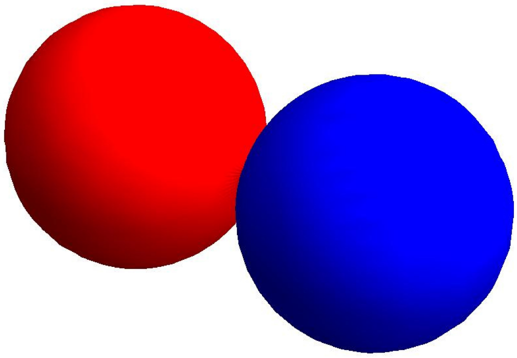


Fig.XX.It shows separate NPS composed of two distinct elements. The parameters to be specified are: (I) radius of one of the two elements, (ii) global stoichiometry, and (iii) the distance between these NPS, keeping in mind that they can not overlap.

1.4) Octahedric NP

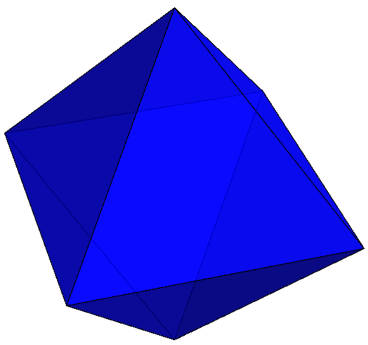


Fig. XX it shows an octahedric NP. The parameters to be specified are:..

1.5) Triangular Plate NP

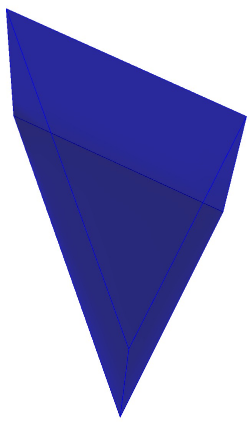


Fig. XX. It shows a triangular NP. The parameters to be specified are:

1.6) Ellipsoidal NP

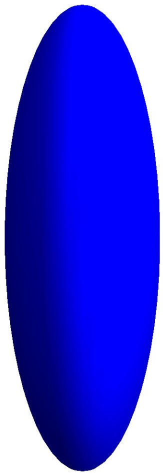


Fig. XX. It shows an ellipsoidal NP. The parameters to be specified are: (i) x-length, (ii) y-length, (iii) z-length.

Here ellipsoids can be created straightforwardly.

Prolate and oblate ellipsoids can be generated as shown in Fig. XX.

1.7) Many-shell NP

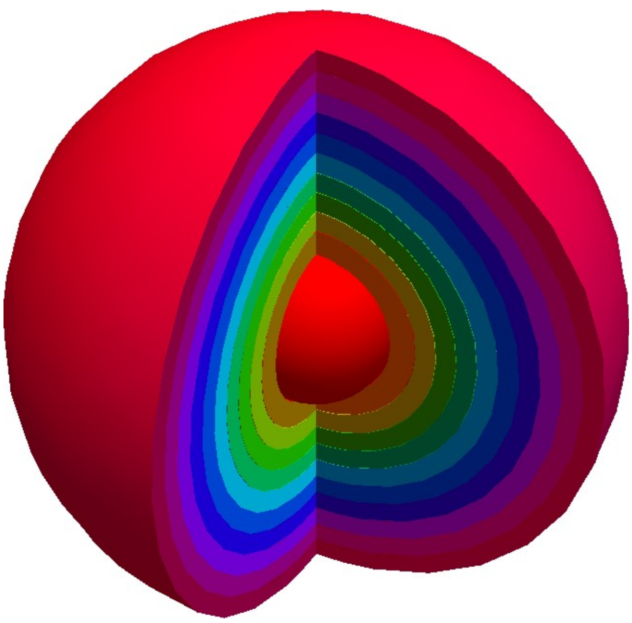


Fig. XX. It shows a spherical NP composed of many concentrically segmented spherical shells.

The idea in this shape configuration is to segment the spherical NP into many concentric shell according to user`s will. This can be of great importance regarding a depth-profile in the NP, where the concentration of a specific element can vary radially according to a specific law.
In this geometry, it can be specified the number of parts and the initial index.

1.8) Cubic NP

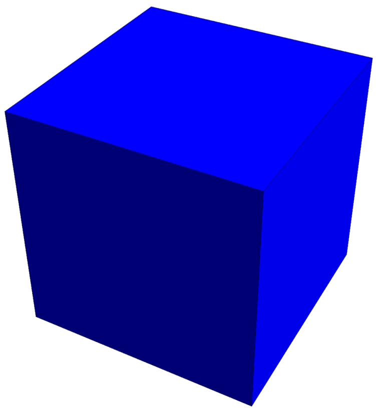


Fig. XX. It shows a cubic NP. The parameters to be specfied are just the cube edge length

1.9.1) Pyramidal NP

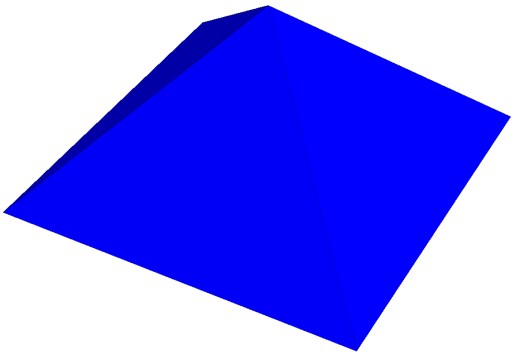


Fig. XX. It shows a
pyramidal NP.

The parameters to be specified are: (I) base-length, and (ii) z-height.

1.10.1) Spherical NP with small NPs on its surface

incoreshell_spheresurface

The parameters to be specified are:

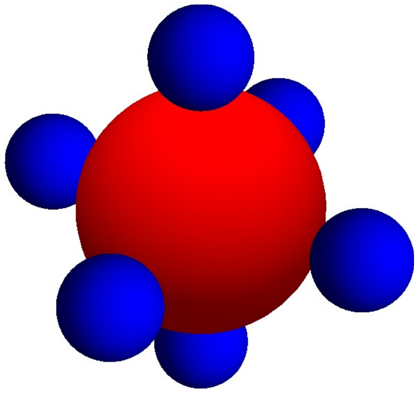


Fig. XX. It shows a NP composed of a core@shell NP with smaller NPs on its surface.

1.10.2) Spherical NP with small NPs on its surface

incoreshell_spheresurfacetwo

The parameters to be specified are:

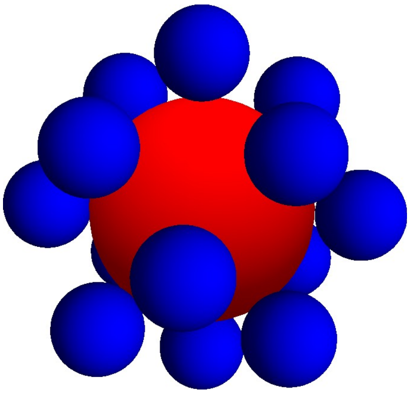


Fig. XX. It shows a NP composed of a core@shell NP with smaller NPs on its surface.

1.11) Paving Stone NP

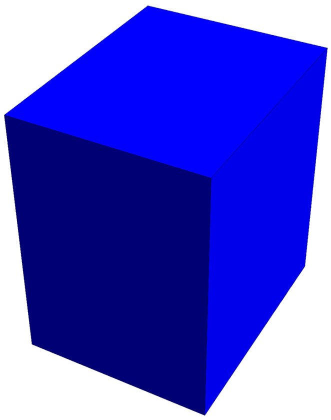


Fig. XX. It shows a Paving Stone-shaped NP. The parameters to be specified are: (i) x-length, (ii) y-length, and (iii) z-length.

1.12) Semi-Spherical NP

FOI!!!

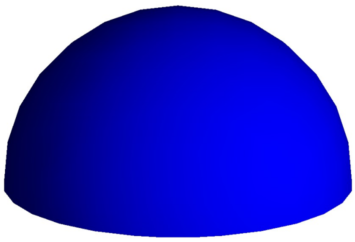


Fig. XX. It is shown a semi-spherical NP.

1.13) Hemispherical NP

FOI!!!!!!

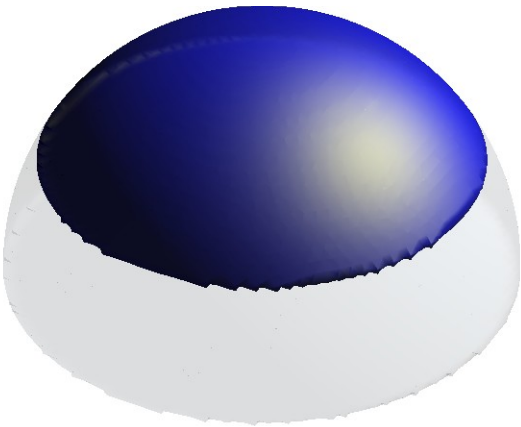


Fig. XX. It is shown a hemispherical NP., along with its whole semi-spherical part in transparent color.

1.14) Pill-form NP

FOI!!!!!

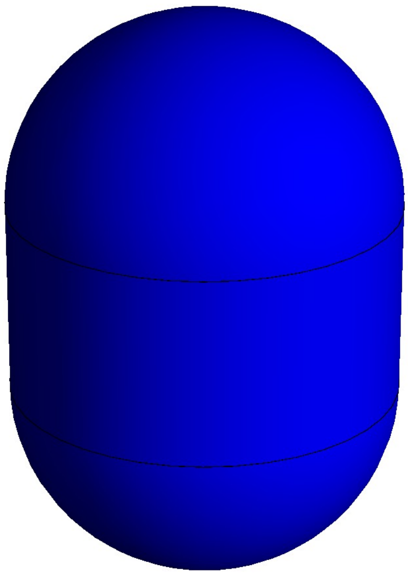


Fig. XX. It shows a NP with a pill shape

The parameters to be specified are:

1.15) Cylindrical NP

This shape consists of a cylindric NP.

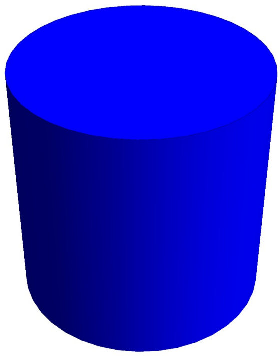


Fig. XX. It is shown a cylindrical NP. The parameters to be chosen are: (I) the basal radius and (ii) height.

1.16) Conic NP

This shape consists of a conic NP
with core@shell structure

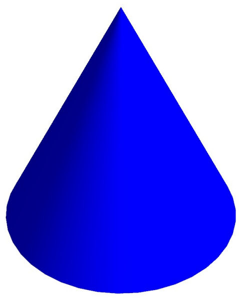


Fig. XX. It is shown a conic NP.

Parameters to be specified:

conicradius1 (coreradius) = ;
conicradius2 (shellradius) = ;
conicheight1 (height of the first part) = ;
conicheight2 (height of the second part) = ;

1.2) Depth Profiling Structures

The aim of this section is to use certain structures of the following subsection and to create matrices in order to be possible to realize depth profile in such NP structures.

Maybe this must appear in the second version.

2) Piling structures

Herein are shown some piling structures that can be chosen.
The parameters must be specified, requiring mainly the following: “shape”, “NP dimensions”, “sizes of matrix construction”.

2.1) Rectangular and Cubic Piling

Number of layers allowed: **unlimited**

2.1.1) Spheric Rectangular Piling

In Fig. XX is shown a spheric cubic piling structure.

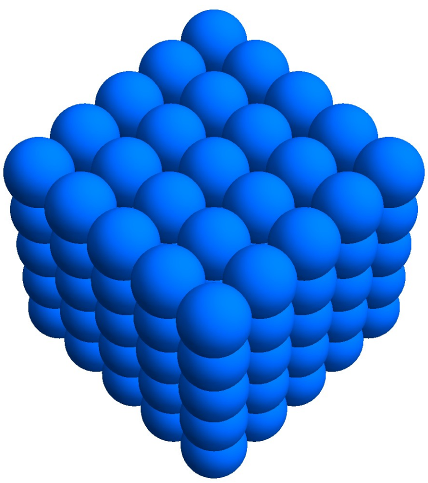


Fig. XX. It is shown a cubic piling structure composed of spheres

In Fig. XX is shown a spheric rectangular piling structure.

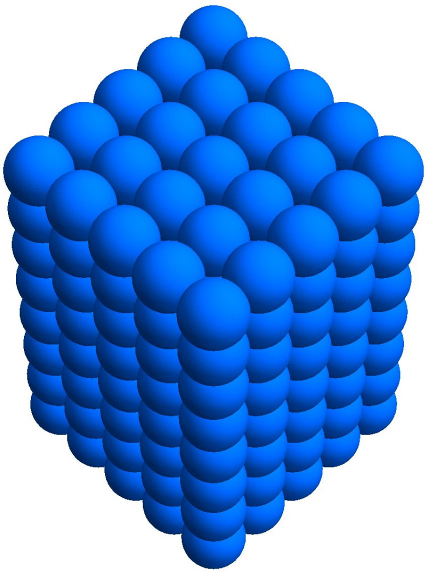


Fig. XX. It is shown a rectangular piling structure composed of spheres

2.1.1) Cubic Rectangular Piling

In Fig. XX is shown a cubic cubic piling structure.

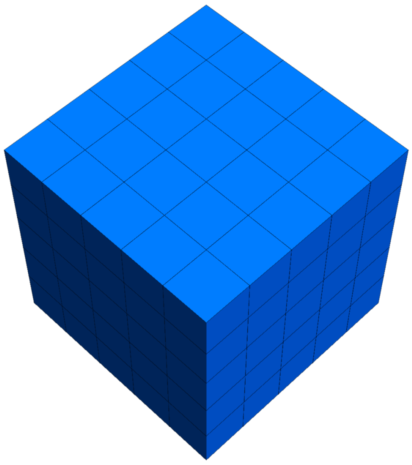


Fig. XX. It is shown a cubic piling structure composed of cubes.

In Fig. XX is shown a cubic rectangular piling structure.

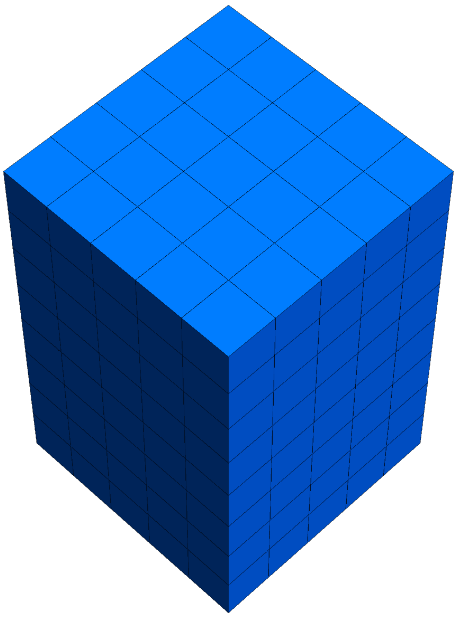
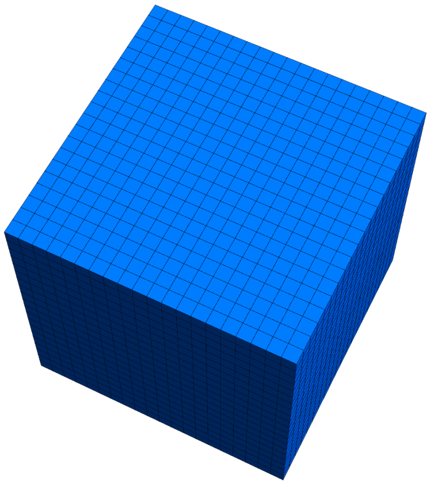


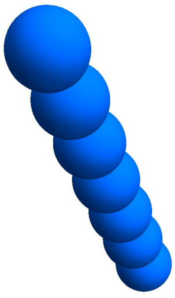
Fig. XX. It is shown a rectangular piling structure composed of cubes.



2.2) Column Piling

Number of layers allowed: **unlimited**

In Fig. XX, it is shown the construction of column piling with a height specification of 8 layers.

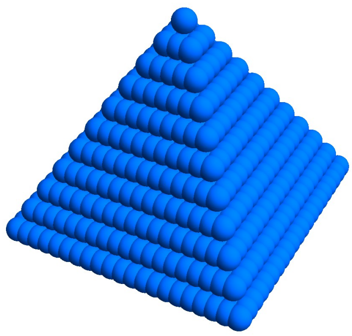


2.3) Pyramidal Piling

In this section are the types of piling forming a pyramid for some structures, along with the parameters needed to generate these matrices.

2.3.1) Spheric Pyramidal Piling

Number of layers allowed: **unlimited**



For instance, in MtxGen a pyamid of 20 layers (Fig. XX) can also be generated, depending mainly on the computer memory

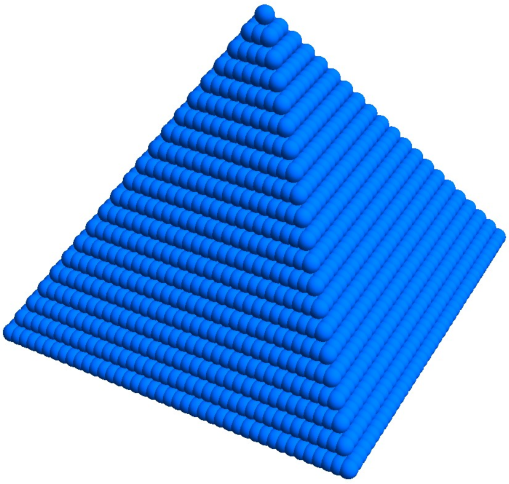
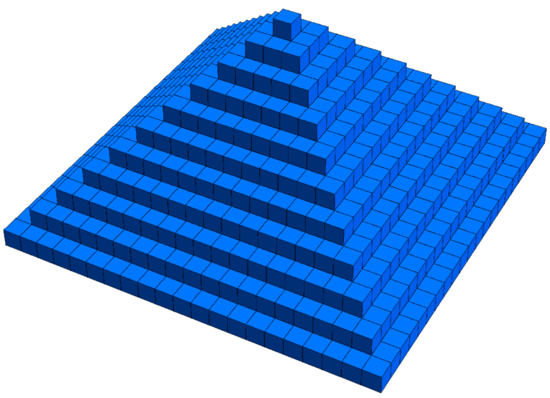


Fig XX. It is shown a pyramid composed of 20 layers with a pyramidal basis of 20x20 spherical particles. It is noteworthy that in this geometry 2870 spheres are agglomerated, forming a pyramidal structure.

2.3.2) Cubic Pyramidal Piling

Number of layers
allowed: **unlimited**



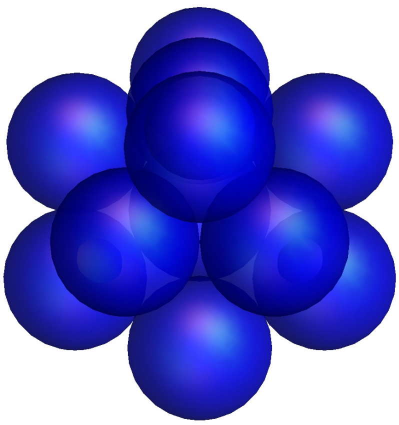
2.4) Hexagonal Piling

In this section are shown the piling structures with some hexagonal geometry that can be constructed, along with the parameters needed to generate it.
In these structures, there is a number of layers that is allowed.
Larger values than the allowed values of the z matrix height will not produce any modification in the final matrix output, just more 0's, whereas shorter values than the allowed values will produce the desired layer of such matrix.

In the following are specified the hexagonal piling geometries, along with a figure showing its geometric shape.

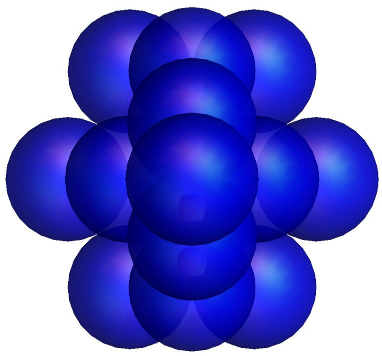
2.4.1) HEX1

Number of layers allowed: **3**



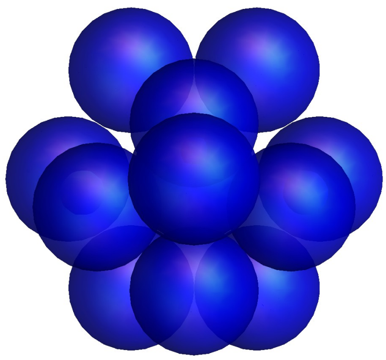
2.4.2) HEX2

Number of layers allowed: **4**



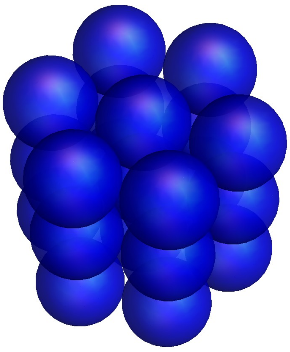
2.4.3) HEX3

Number of layers allowed: **3**



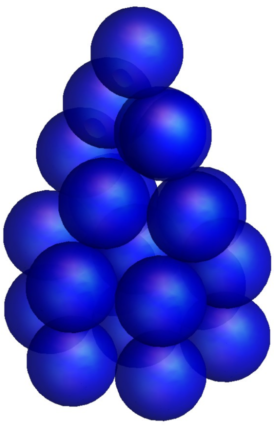
2.4.4) HEX4

Number of layers allowed: **3**



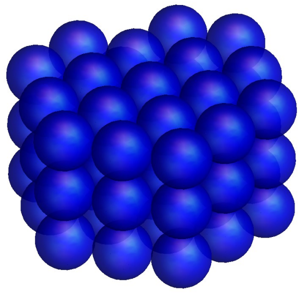
2.4.5) HEX5

Number of layers allowed: **5**



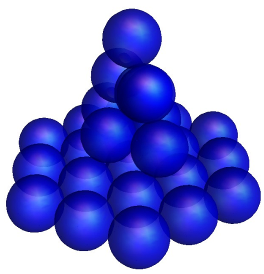
2.4.6) HEX6

Number of layers allowed: **3**



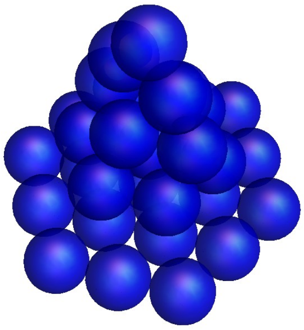
2.4.7) HEX7

Number of layers allowed: **4**



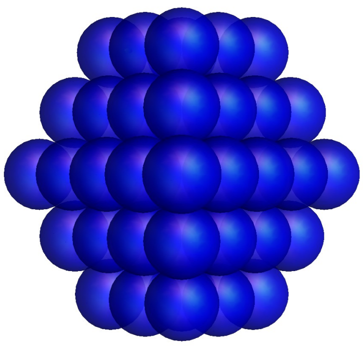
2.4.8) HEX8

Number of layers allowed: **5**



2.4.9) HEX9

Number of layers allowed: **5**



2.4.10) Hexagonal layer

Number of layers allowed: **unlimited**

2.4.11) Hexagonal Pyramid

Number of layers allowed: **unlimited**

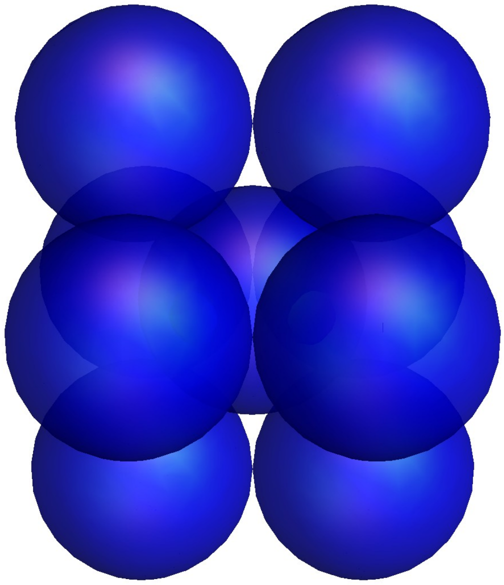
2.5) Triangular Piling

Number of layers allowed: **unlimited**

2.6) Jonder Piling

2.6.1) Jonder Struct 1

To generate such a structure, the number of layers must be specifed as 3.



2.5.2) Jonder Struct 2

To generate such a structure, the number of layers must be specifed as 3.