Structure and Morphology of Crystalline Metal Nanoparticles: Polyhedral Cubic Particles

Klaus E. Hermann

Inorg. Chem. Dept., Fritz-Haber-Institut der Max-Planck-Gesellschaft,
Faradayweg 4-6, 14195 Berlin, Germany.

Abstract

We examine nanoparticles (NPs) forming polyhedral sections of the ideal cubic lattice, simple (sc), body centered (bcc), and face centered (fcc) cubic, which are confined by facets characterized by densest and second densest $\{h\,k\,l\}$ monolayers of the lattice. Together with the constraint that the NPs exhibit the same point symmetry as the ideal cubic lattice, i.e. O_h, different types of generic NPs serve for the definition of general polyhedral cubic NPs. Their structural properties, such as shape, size, and surface facets, are discussed in analytical and numerical detail with visualization of characteristic examples. The geometric relationships of the model particles expressed by corresponding formulas and numerical tables can be used to estimate shapes and sizes of real compact metal nanoparticles observed by experiment.

I. Introduction

Nanoparticles of many sizes, shapes, and composition have become the target of a large number of recent experimental and theoretical studies due to their exciting physical and chemical properties [a1]. Here we mention only important applications in medicine [a2] or in catalysis where catalytic metal nanoparticles have become ubiquitious [a3, a4].

Shapes of real metal nanoparticles (NP), observed by experiment, are determined by their individual atoms being exposed to different local environments depending on their location inside the particle. Metal atoms close to the particle surface experience fewer atom neighbors compared to those inside the particle volume. This influences their interatomic binding and affects the particle structure. The variation of atom environments in finite particles depends strongly on the particle size since the relative number of surface atoms compared with those of the inner particle core becomes smaller with increasing size. This suggests that deviations from a crystalline bulk structure with its equivalent atom centers arranged in three-dimensional periodicity become less important as the particle size increases.

In many cases, structural properties of metal NPs with only a few atoms do not reflect those of corresponding bulk crystals. Details depend on the specific cluster shape and elemental composition and there are no general guidelines as to interatomic distances or angles or as to symmetry. This is illustrated by theoretical studies on silver NPs up to Ag_{12} [a5] where equilibrium structures are found to deviate substantially from those of sections of the face-centered cubic crystal describing bulk silver. Also these very small NPs offer different stable isomers with varying shape and structure [a5]. Larger compact metal NPs can also exhibit symmetry properties which are not compatible with those of bulk crystals. As examples, many alkaline earth and transition metal (Nickel, Cobalt) NPs in gas phase with up to 5000 atoms [a6, a7] are believed to form compact particles with icosahedral symmetry I_h which cannot appear in perfect bulk crystals due to their 5-fold rotational axes. Their structure can be explained by the concept of polyhedral atom shell filling which yields preferred NP sizes connected with so-called magic numbers of atoms [a7, a8]. However, many metal NPs have been observed by experiment to exhibit cubic O_h symmetry which can be associated with compact sections of cubic bulk crystal structures, both face- and body-centered cubic, or can be approximated accordingly [a9]. Here examples are Aluminum and Indium NPs in gas phase between 1000 and 10000 atoms [a6] which are suggested to form compact polyhedral particles of face-centered cubic structure where confining facets are described by sections of densest (low Miller index) monolayers referring to $\{h\,k\,l\}$ families. Amongst these cuboctahedral shapes enclosed by both triangular $\{1\,1\,1\}$ and square

{1 0 0}facets, have been discussed. The corresponding NPs represent a fairly good approximation to spherical NPs since the atoms of the different planar sections do not vary too much in their distance from the NP center. Also other high-symmetry structures representing compact sections of face-centered cubic bulk crystals have been proposed in the literature [a6, a7] as possible structures of compact metal NPs where we mention only octahedral NPs which will be discussed below. Finally, metal NPs of O_h symmetry described by sections of body-centered cubic bulk crystals have been suggested in the literature [a6, a10]. Here theoretical structure studies can help to describe and classify ideal compact cubic nanoparticles and, thus, identify structural properties of many real metal nanoparticles.

In this work we examine ideal nanoparticles forming polyhedral sections of the ideal cubic lattice, simple (sc), body centered (bcc), and face centered (fcc) cubic. These particles are assumed to be confined by facets of densest and second densest monolayers described by Miller indexed $\{h\,k\,l\}$ families, i.e. {1 0 0}, {1 1 0} for sc and bcc as well as {1 1 1}, {1 0 0} for fcc. Together with the constraint that the NPs exhibit the same point symmetry as the ideal cubic lattice, i.e. O_h, there are different types of generic NPs which serve for the definition of general polyhedral NPs. Their structural properties , such as shape, size, and surfaces, are discussed in analytical and numerical detail with visualization of characteristic examples. These results can also be used as a repository for structures of compact NPs with internal cubic lattice. All NP graphics and analyses have been obtained with the help of the Balsac software developed by the author [a11].

II. Results and Discussion

A. Nanoparticles with Simple Cubic (sc) Lattice Structure

The simple cubic (sc) lattice is defined by lattice vectors $\underline{R}_1$, $\underline{R}_2$, $\underline{R}_3$ in Cartesian coordinates according to

$$\underline{R}_1 = a(1,0,0) \ , \quad \underline{R}_2 = a(0,1,0) \ , \quad \underline{R}_3 = a(0,1,0) \tag{A.1}$$

where a is the lattice constant. The three densest monolayer families of the sc lattice are described by six square shaped $\{1\,0\,0\}$ (highest density), twelve rectangular $\{1\,1\,0\}$, and eight hexagonal $\{1\,1\,1\}$ netplanes where distances between adjacent parallel netplanes are given by

$$d_{\{100\}} = a \ , \quad d_{\{110\}} = a/\sqrt{2} \ , \quad d_{\{111\}} = a/\sqrt{3} \tag{A.2}$$

The point symmetry of the sc lattice is characterized by O_h with symmetry centers at all atom sites and at the void centers of each elementary cell.

Compact simple cubic nanoparticles (NPs) are confined by finite sections of monolayers (facets) whose structure is described by different netplanes $(h\,k\,l)$. If they exhibit central O_h symmetry and show an $(h\,k\,l)$ oriented facet they must must also include all other symmetry related facets characterized by orientations of the complete $\{h\,k\,l\}$ family. Thus, general sc NPs of O_h symmetry are determined by facets whose orientation can be defined by those of different $\{h\,k\,l\}$ families. (As an example, we mention the $\{1\,0\,0\}$ family with its six netplane orientations $(\pm1\,0\,0)$, $(0\,\pm1\,0)$, $(0\,0\,\pm1)$.) Further, according to the symmetry of the sc host lattice possible NP centers can only be atom or O_h symmetry void sites of the lattice. This will be discussed at different levels of complication in the following.

A.1. Generic sc Nanoparticles

First, we consider generic sc nanoparticles (NPs) of O_h symmetry which are confined by facets with orientations of only one netplane family $\{h\,k\,l\}$. This allows to distinguish between different generic NP types where we focus on those confined by $\{1\,0\,0\}$ or $\{1\,1\,0\}$ facets which correspond to the densest monolayers of the sc lattice and offer the flattest NP facets.

(a) **Generic cubic** sc NPs, denoted **sc[N, 0)** (the notation of sc NPs, in particular the bracketing, will be explained in Secs. A.2, 3), contain an **atom** at their symmetry center for **even** N and a **void** for **odd** N. They are confined by all six $\{1\,0\,0\}$ monolayers with distances $D_{\{100\}} = N\,d_{\{100\}}$ between parallel monolayers (polyhedral NP diameters). This yields six

square shaped {1 0 0} facets with $(N + 1)$ edge atoms each and eight polyhedral atom corners, see Fig. A.1.
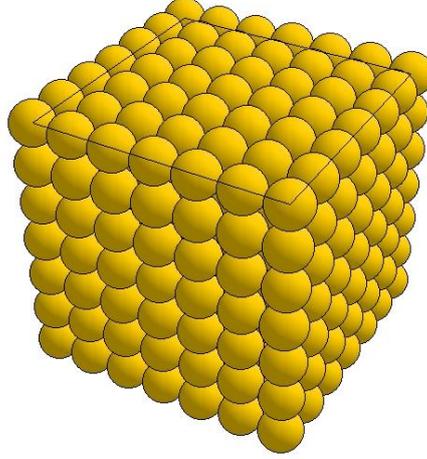
Figure A.1. Atom ball models of a generic cubic sc NP, sc[6, 0) with an atom at its center. The black lines sketch the square {1 0 0}facet shapes.

(b) **Generic rhombic** sc NPs are confined by all twelve {1 1 0} monolayers with distances $D_{\{110\}} = 2M\, d_{\{110\}}$ between parallel monolayers (polyhedral NP diameters). Here we distinguish two NP types.

Generic rhombic A sc NPs, denoted **sc(0, M]**, contain an **atom** at their symmetry center and are confined by rhombic facets of all twelve {1 1 0} monolayers, see Figs. A.2. For even M, Fig. A.2a, the {1 1 0} rhombi contain $(M + 1)$ parallel nearest neighbor atom rows of increasing/decreasing length in the sequence 0 (atom), $2a$, …, $M\,a$, …, $2a$, 0 (atom). For odd M, Fig. A.2b, the lengths increase/decrease in the sequence 0 (atom), $2a$, …, $(M$-$1)a$, $(M$-$1)a$, …, $2a$, 0 (atom). This yields a capping of the rhombi at their near corners resulting in eight additional triangular {1 1 1} microfacets at the sc NP surface. Altogether, the generic rhombic A sc NPs are described as rhombic dodecahedra offering 14 polyhedral atom corners for even M and reminding of the shape of Wigner-Seitz cells of the face centered cubic (fcc) crystal lattice [a12]. For odd M, the dodecahedra are capped at eight corners which leads to 30 polyhedral atom corners.
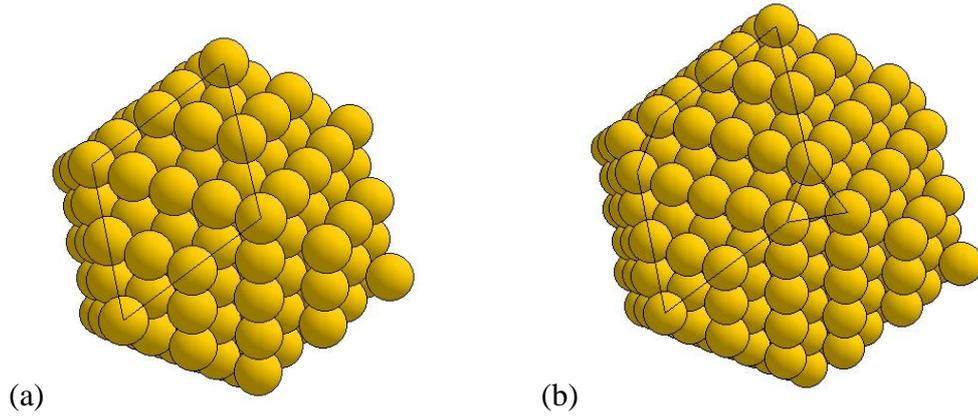
Figure A.2. Atom ball models of generic rhombic A sc NPs with an atom at their symmetry centers, (a) sc(0, 4] and (b) sc(0, 5]. The black lines sketch the (capped) rhombic {1 1 0} and triangular {1 1 1} facet shapes.

Generic rhombic B fcc NPs, denoted **sc(1, M]**, contain a **void** at their symmetry center and are also confined by rhombic facets of all twelve {1 1 0} monolayers, see Figs. A.3. For even M, Fig. A.3a, the {1 1 0} rhombi contain M parallel nearest neighbor atom rows of increasing/decreasing length in the sequence a, $3a$, …, $(M-1)a$, $(M-1)a$, …, $3a$, a. This yields a capping of the rhombi at their far corners resulting in six additional square {1 0 0} microfacets at the sc NP surface. For odd M, Fig. A.3b, the lengths increase/decrease in the sequence a, $3a$, …, $M a$, …, $3a$, a which yields a capping of the rhombi at all four corners resulting in eight additional triangular {1 1 1} microfacets. Altogether, the generic rhombic B sc NPs are described by capped rhombic dodecahedra offering 48 (32) polyhedral atom corners for even (odd) M and.
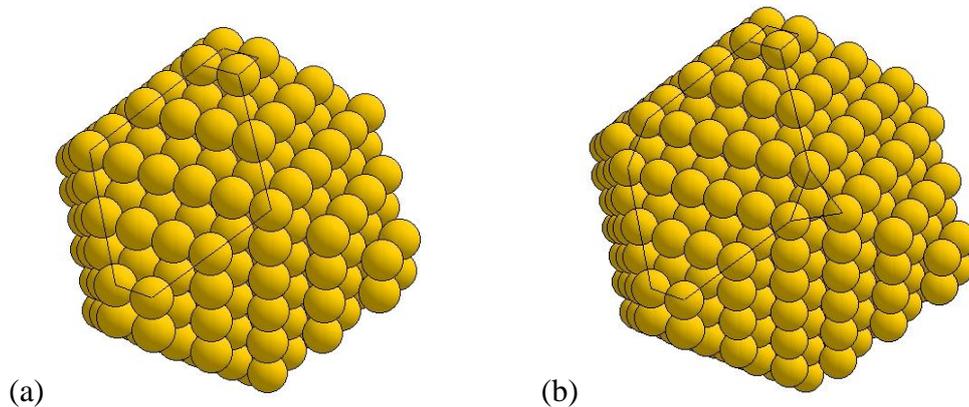
Figure A.3. Atom ball models of generic rhombic B sc NPs with a void at their symmetry centers, (a) sc(1, 5] and (b) sc(1, 6]. The black lines sketch the (capped) rhombic {1 1 0}, the triangular {1 1 1}, and the square {1 0 0} facet shapes.

A.2. Non-generic sc Nanoparticles

Non-generic sc nanoparticles of O_h symmetry are confined by facets with orientations of several netplane families $\{h_i\,k_i\,l_i\}$. This can be considered as combining the confinements of the corresponding generic NPs, NP_i, determined by $\{h_i\,k_i\,l_i\}$ with suitable polyhedral diameters, sharing their symmetry center and type (atom or void). As an example we discuss non-generic sc nanoparticles which combine two generic nanoparticles NP_1, NP_2 of the types detailed in Sec. A.1. Thus, the resulting sc NP contains only atoms inside both partner NPs. Here three possible scenarios can be distinguished, nanoparticle NP_2 contains all atoms of NP_1 (yielding generic NP_1), NP_1 contains all atoms of NP_2 (yielding generic NP_2), or NP_1 and NP_2 share only parts of their atoms (intersecting, which yields true non-generic NPs). These scenarios are determined by the choice of the two netplane families $\{h\,k\,l\}$ and by relationships between the corresponding polyhedral NP diameters $D_{\{hkl\}}$ defined by N and M. In the following, we restrict ourselves to non-generic sc NPs defined by pairs of generic cubic and rhombic NPs.

Non-generic sc NPs with an **atom** at their symmetry center combine a generic cubic NP, sc[N, 0) with even N, and a rhombic A NP, sc(0, M] where polyhedral diameters amount to

$$D_{\{100\}} = N\,d_{\{100\}} = N\,a, \ \text{N even}, \qquad D_{\{110\}} = 2M\,d_{\{110\}} = 2M\,a/\sqrt{2} \qquad (A.3)$$

Thus, the smallest rhombic A NP which surrounds the cubic NP is defined with (A.2) by

$$D_{\{110\}} = \sqrt{2}\,D_{\{100\}} \quad \text{and hence} \quad M = N \qquad (A.4)$$

On the other hand, the smallest cubic NP which surrounds the rhombic A NP is defined with (A.2) by

$$D_{\{100\}} = \sqrt{2}\,D_{\{110\}} \quad \text{and hence} \quad N = 2M \qquad (A.5)$$

As a consequence, non-generic sc NPs with an atom at their symmetry center combining generic cubic and rhombic A NPs, NP_1, NP_2, yield the choices shown in Table A.1.

NP_1 / NP_2	NP_1 in NP_2	NP_2 in NP_1
Cubic / Rhombic A sc[N, 0) / sc(0, M], N even	$M \geq N$	$N \geq 2M$

Table A.1. Constraints of structure parameters N, M for pairs of sc NPs, NP_1 and NP_2, sharing an atom as their symmetry center.

Non-generic sc NPs with a **void** at their symmetry center combine a generic cubic NP, sc[N, 0) with odd N, and a rhombic B NP, sc(1, M] where polyhedral diameters amount to

$$D_{\{100\}} = N\, d_{\{100\}} = N\, a, \ \ \text{N odd}, \ \ \ D_{\{110\}} = 2M\, d_{\{110\}} = 2M\, a/\sqrt{2} \tag{A.6}$$

which also leads to relation (A.4) for the smallest rhombic B NP surrounding the cubic NP. Further, the smallest cubic NP which surrounds the rhombic B NP is given by

$$(D_{\{100\}} + d_{\{100\}}) = \sqrt{2}\, D_{\{110\}} \ \ \ \ \text{and hence} \ \ \ \ N = 2M - 1 \tag{A.7}$$

Therefore, non-generic sc NPs with a void at their symmetry center combining generic cubic and rhombic B NPs, NP_1, NP_2, yield the three choices shown in Table A.2.

NP_1 / NP_2	NP_1 in NP_2	NP_2 in NP_1
Cubic / Rhombic B sc[N, 0) / sc(1, M], N odd	$M \geq N$	$N \geq 2M\text{-}1$

Table A.2. Constraints of structure parameters N, M for pairs of sc NPs, NP_1 and NP_2, sharing a void as their symmetry center.

Tables A.1, 2 show in particular that true non-generic sc NPs, defined by pairs of generic cubic NPs, sc[N, 0), and rhombic NPs, sc(q, M], $q = 0, 1$, refer to structure parameters N, M which bracket each other according to

$$M < N < 2M \ , \ \ \ \ N/2 < M < \text{N} \ \ \ \ \ \ \ \ \ \ \text{N even, atom centered} \tag{A.8a}$$

$$M < N < 2M - 1 \ , \ \ \ \ (N+1)/2 < M < \text{N} \ \ \ \ \ \ \ \text{N odd, void centered} \tag{A.8b}$$

These non-generic sc NPs may be called **cubo-rhombic** and denoted as **sc[N, M]** combining a generic cubic sc[N, 0) (first index) with a rhombic NP (second index) where the latter is rhombic A, sc(0, M], for even N and rhombic B, sc(1, M], for odd N. The nomenclature together with the results of Tables A.1, 2 suggests an alternative notation for generic NPs where we may formally write

$$\text{generic cubic} \ \ \ \ \ \ \ \ \text{sc[N, 0)} \ = \ \text{sc[N, M]} \ , \ \ \ \ \ \ \ \ \ \ \ N \leq M \tag{A.9a}$$

$$\text{generic rhombic A} \ \ \ \text{sc(0, M]} \ = \ \text{sc[N, M]} \ , \ \ \ \ \ \ \ \ \ \ \ N \geq 2M \tag{A.9b}$$

$$\text{generic rhombic B} \ \ \ \text{sc(1, M]} \ = \ \text{sc[N, M]} \ , \ \ \ \ \ \ \ \ \ \ \ N \geq 2M - 1 \tag{A.9c}$$

A.3. Cubo-rhombic sc Nanoparticles

In the following we will discuss the detailed structure of true cubo-rhombic NPs sc[N, M] determined by corresponding structure parameters N, M and confined by the two densest monolayer

families {1 0 0} and {1 1 0}. These NPs contain an **atom** at there symmetry center for **even** N while their symmetry center is **void** for **odd N**.

First, we consider **atom centered** sc NPs. Starting from a generic cubic NP sc[N, 0) (N even) with a polyhedral NP diameter $D_{\{100\}} = N\, d_{\{100\}}$ the smallest enclosing rhombic A NP sc(0, M] has a polyhedral NP diameter $D_{\{110\}} = 2M\, d_{\{110\}}$ with $M = N$ according to Tables A.1, 2. Shrinking the rhombic sc NP, i.e. for smaller M values given by $M = N - m$, $m \geq 0$, the cubic and rhombic sc NPs intersect yielding a **cubo-rhombic A** NP sc[N, $M = N - m$]. In the following we define this NP by **sc[N, m)** which is compatible with the initial definition of a generic cubic sc NP denoted sc[N, 0) in Sec. A.1. The constraints on M given in Table A.1 can be expressed by equivalent constraints on m yielding

$$N/2 \leq M \leq N \;, \qquad\qquad 0 \leq m \leq N/2 \qquad\qquad \text{cubo-rhombic A} \qquad\qquad \text{(A.10)}$$

where m values larger than $N/2$ result in generic rhombic A sc NPs. The building scheme corresponds to the generic cubic NP sc[N, 0) being truncated at its twelve edges by removing m {1 1 0} facet layers each.

On the other hand, starting from a generic rhombic A NP sc(0, M] with a polyhedral NP diameter $D_{\{110\}} = 2M\, d_{\{110\}}$ the smallest enclosing cubic sc NP has a polyhedral NP diameter $D_{\{100\}} = N\, d_{\{100\}}$ with $N = 2M$ according to Table A.1. Shrinking the cubic sc NP, i.e. for smaller N values given by $N = 2M - n$ with $n = 0, 2, 4 \ldots$ the cubic and rhombic NPs intersect yielding also a **cubo-rhombic A** NP sc[$N = 2M - n$, M]. In the following we define this NP by **sc(n, M]** with even n which is compatible with the initial definition of a generic rhombic A sc NP denoted sc(0, M] in Sec. A.1. The constraints on N given in Table A.1 can be expressed by equivalent constraints on n yielding

$$M \leq N \leq 2M \;, \qquad\qquad 0 \leq n \leq M , \quad n \text{ even} \qquad\qquad \text{cubo-rhombic A} \qquad\qquad \text{(A.11)}$$

where n values larger than M result in generic cubic sc NPs. The building scheme corresponds to the generic rhombic A NP sc(0, M] being truncated at its six 4-fold symmetry corners by removing $n/2$ {1 0 0} facet layers each.

The two building schemes must yield the same cubo-rhombic A NP sc[N, M] where the two structure parameters N, M quantify the polyhedral NP diameters $D_{\{100\}}$ and $D_{\{110\}}$ according to

$$D_{\{100\}} = N\, d_{\{100\}} \;, \qquad\qquad D_{\{110\}} = 2M\, d_{\{110\}} \qquad\qquad\qquad \text{(A.12)}$$

with the basic netplane distances $d_{\{100\}}$ and $d_{\{110\}}$ given by (A.2). Further, the relations

$$M = N - m \;, \qquad\qquad N = 2M - n \;, \quad n \text{ even} \qquad\qquad\qquad \text{(A.13a)}$$

from the two building schemes can be converted to

$$n = 2M - N \ , \qquad\qquad m = N - M \qquad\qquad\qquad (A.13b)$$

$$N = n + 2m \ , \qquad\qquad M = n + m \qquad\qquad\qquad (A.13c)$$

Next, we consider **void centered** sc NPs whose treatment is completely analogous to the atom centered case. Starting from a generic cubic NP sc[N, 0) (N odd) and its smallest enclosing rhombic B NP sc(1, M] with $M = N$, shrinking the rhombic sc NP yields a **cubo-rhombic B** NP sc[N, $M = N - m$] which can be defined by **sc[N, m)**. The constraints on M given in Table A.2 can be expressed by equivalent constraints on m yielding

$$(N+1)/2 \le M \le N \ , \qquad 0 \le m \le (N - 1)/2 \qquad \text{cubo-rhombic B} \qquad (A.14)$$

where m values larger than $(N - 1)/2$ result in generic rhombic B sc NPs. The building scheme corresponds also to the generic cubic NP sc[N, 0) being truncated at its twelve edges by removing m {1 1 0} facet layers each.

On the other hand, starting from a generic rhombic B NP sc(1, M] and its smallest enclosing cubic sc NP sc [N, 0) with $N = 2M - 1$, shrinking the cubic sc NP yields also a **cubo-rhombic B** NP sc[$N = 2M - n$, M] which can be defined by **sc[n, M)** with odd n. This includes the initial definition of a generic rhombic B sc NP denoted sc(1, M]. The constraints on N given in Table A.2 can be expressed by equivalent constraints on n yielding

$$M \le N \le 2M\text{-}1 \ , \qquad 1 \le n \le M \ , \quad n \text{ odd} \qquad \text{cubo-rhombic B} \qquad (A.15)$$

where n values larger than M result in generic cubic sc NPs. The building scheme corresponds to the generic rhombic B NP sc(1, M], being truncated at its six 4-fold symmetry corners by removing $(n - 1)/2$ {1 0 0} facet layers each.

The two building schemes must yield the same cubo-rhombic B NP sc[N, M] resulting in

$$M = N - m \ , \qquad\qquad N = 2M - n \ , \quad n \text{ odd} \qquad\qquad (A.16)$$

and hence to relations (A.13b), (A.13c) derived above.

Altogether, relations (A.13) suggest an alternative set of structure parameters n, m which characterize the deviation of the cubo-rhombic NP sc[N, M] from its generic envelope NPs, cubic sc[N, 0) and rhombic A sc(0, M] or rhombic B sc(1, M]. Thus, **cubo-rhombic A** (atom centered) or **B** (void centered) NPs can also be denoted **sc(n, m)** with even or odd n, respectively.

The structure parameters n, m are also connected with geometric properties of the NP facets, in particular, with characteristic lengths of the facet edges. The cubo-rhombic sc NPs, sc[N, M] $\equiv$

sc(n, m), are confined by all six {1 0 0} facets of square shape with ($n + 1$) × ($n + 1$) atoms each and by all twelve {1 1 0} facets, see Figs. A.4. For even m, Fig. A.4a, the {1 1 0} facets are hexagonal and contain $m + 1$ parallel nearest neighbor atom rows of increasing/decreasing length in the sequence $n\,a$, $(n+2)a$, …, $(n + m)\,a$, …, $(n+2)a$, $n\,a$. For odd m, Fig. A.4b, the {1 1 0} facets are capped hexagonal (octagonal) and the lengths of the $m + 1$ atom rows increase/decrease in the sequence $n\,a$, $(n+2)a$, …, $(n + m -1)a$, $(n + m -1)a$, …, $(n+2)a$, $n\,a$. This yields eight additional triangular {1 1 1} microfacets shown in Fig A.5b. Altogether, the sc NPs are described by cubo-rhombic polyhedra offering 32 ($n > 0$, $m > 0$, m even) or 48 ($n > 0$, $m > 0$, m odd) corners with true cubic ($n > 0$, $m = 0$, eight corners) and true rhombic A ($n = 0$, $m > 0$, 14 corners) being special cases.

(a)   (b)
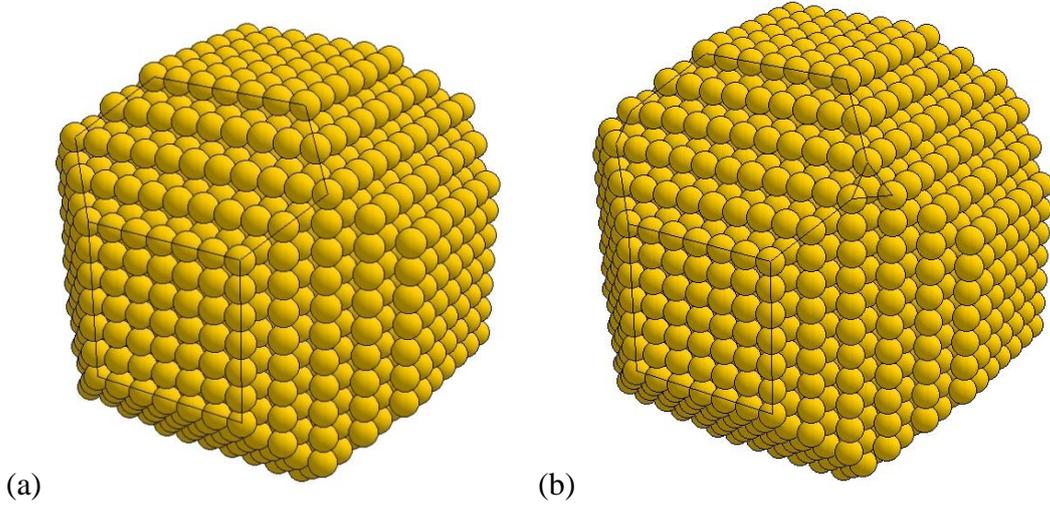
Figure A.4. Atom ball models of atom centered cubo-rhombic A sc NPs, (a) sc[14, 10] ≡ sc(6, 4) and (b) sc[16, 11] ≡ sc(6, 5). The black lines sketch the square {1 0 0}, (capped) hexagonal {1 1 0} and triangular {1 1 1} facet shapes.

The confinement of a cubo-rhombic A sc[N, M] ≡ sc(n, m) NP with an atom at its symmetry center (N, n even) by its generic envelope sc NPs, cubic sc[N, 0] and rhombic A sc[0, M] with N, M defined by A.13, is illustrated in Fig. A.5 for sc[14, 10] ≡ sc(6, 4) with sc[14,0] and sc(0, 10] forming the envelope sc NPs.
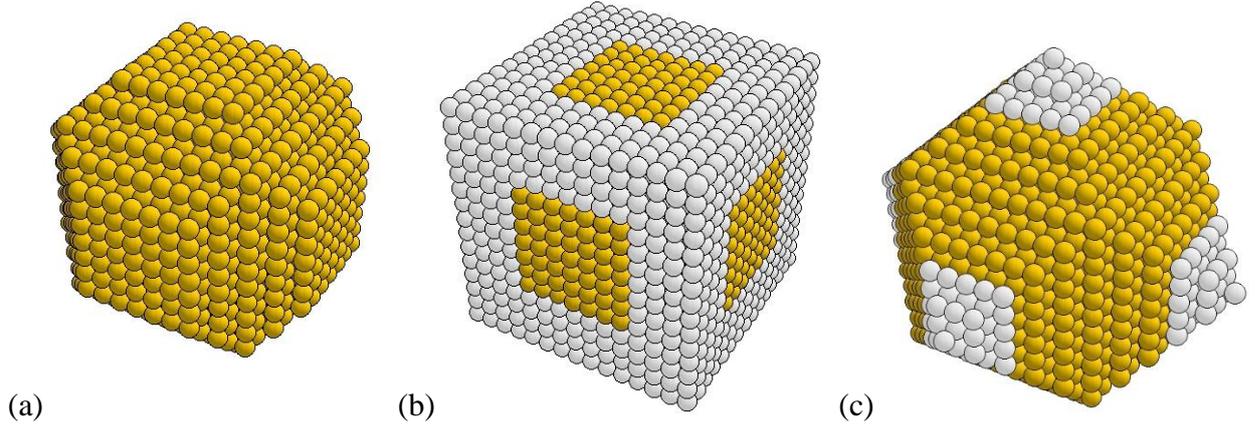
Figure A.5. Atom ball models of a cubo-rhombic A sc[14, 10] ≡ sc(6, 4) NP with its confining generic cubic and rhombic A NPs. (a) Initial sc(6, 4) shown by yellow balls, (b) sc(6, 4) inside generic sc[14, 0], and (c) sc(6, 4) inside generic sc(0, 10). The atoms outside sc(6, 4) are shown by white balls.

Further, the confinement of a cubo-rhombic B sc[N, M] ≡ sc(n, m) NP with a void at its symmetry center (N, n odd) by its cubic sc[N, 0] and rhombic B sc(1, M] envelope sc NPs is shown in Fig. 6 for sc[13, 9] ≡ sc(5, 4) with sc[13,0] and sc(1, 9] forming the envelopes.
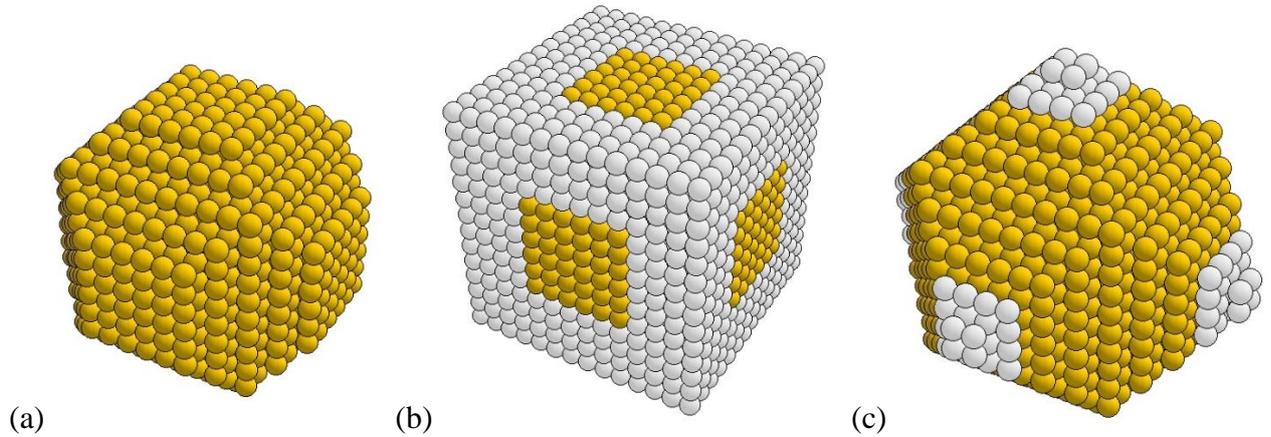
Figure A.6. Atom ball models of a cubo-rhombic B sc[13, 9] ≡ sc(5, 4) NP with its confining generic cubic and rhombic B NPs. (a) Initial sc(5, 4) shown by yellow balls, (b) sc(5, 4) inside generic sc[13, 0], and (c) sc(5, 4) inside generic sc(1, 9]. The atoms outside sc(5, 4) are shown by white balls.

Altogether, the equivalence of structure parameters n, m and N, M according to (A.13) suggests alternative notations of cubo-rhombic sc NPs introduced earlier. Apart from a notation by sc[N, M], meaningful alternatives are sc(n, m), sc[N, m), and sc(n, M] where the different bracketing denotes the different meanings of the two parameters in the notation. Table A.3 lists types

and notations of all cubo-rhombic sc NPs where type A NPs (atom centered) refer to even *n*, *N* values while for type B NPs (void centered) *n*, *N* values are odd.

Type	sc[*N, M*]	sc(*n, m*)	sc[*N, m*]	sc(*n, M*)
Cubo-rhombic A	$M < N < 2M$	$n > 0, m > 0$	$0 < m < N/2$	$0 < n < M$
Cubo-rhombic B	$M < N < 2M$-1	$n > 1, m > 0$	$0 < m < (N$-1$)/2$	$1 < n < M$
Generic cubic	$N = M$	$n > 0, m = 0$	$m = 0$	$n = M$
Generic rhombic A	$N = 2M$	$n = 0, m > 0$	$m = N/2$	$n = 0$
Generic rhombic B	$N = 2M$-1	$n = 1, m > 0$	$m = (N$-1$)/2$	$n = 1$
Elementary cube (B)	$N = M = 1$	$n = 1, m = 0$	$N = 1, m = 0$	$n = M = 1$
Atom (A)	$N = M = 0$	$n = m = 0$	$N = m = 0$	$n = M = 0$

Table A.3. Types and notations of all intersecting and generic sc NPs.

A.4. Properties of Cubo-rhombic sc Nanoparticles

Structural properties characterizing cubo-rhombic sc nanoparticles can be obtained by geometric consideration and simple algebra where we quote only results of the most important quantities. Structure parameters *n*, *m*, *N, M*, according to (A.13), i.e.

$$n = 2M - N \ , \qquad m = N - M \qquad\qquad (A.13b)$$
$$N = n + 2m \ , \qquad M = n + m \qquad\qquad (A.13c)$$

with constraints listed in Tables A.1 - 3 will be used interchangeably and in mixed combinations to simplify formal expressions. Note that according to (A.13) structure parameters *n* and *N* will always be both even or both odd numbers. Results which are valid only for atom centered, type A, or for void centered, type B, sc NPs will be denoted accordingly.

The number of atoms forming an sc(*n, m*) NP are given by the **volume count** denoted $N_{vol}(n, m)$ where simple algebra yields for

- *m* even (*N, M* both even or both odd)

$$N_{vol}(n, m) = (n+m+1)^3 + (n+m+1)(n+m)(n+m-1) - n(n^2-1)$$
$$= (M+1)^3 + M(M^2-1) - (2M-N)\left[(2M-N)^2-1\right] \qquad (A.17a)$$

- **m odd** (*N* even, *M* odd or *N* odd, *M* even)

$$N_{vol}(n, m) = (n+m+1)^3 + (n+m+1)(n+m)(n+m-1) - n(n^2-1) - 1$$
$$= (M+1)^3 + M(M^2-1) - (2M-N)\left[(2M-N)^2-1\right] - 1$$

(A.17b)

with **special cases**

Generic cubic $\qquad N_{vol}(n, 0) = (n+1)^3 = (N+1)^3 \qquad N = n$ (A.18)

Generic rhombic A $\qquad N_{vol}(0, m) = m(2m^2+3m+2)+1$ (A.19a)

$$= M(2M^2+3M+2)+1 \qquad M = m \text{ even}$$

$$N_{vol}(0, m) = m(2m^2+3m+2)$$ (A.19b)

$$= M(2M^2+3M+2) \qquad M = m \text{ odd}$$

Generic rhombic B $\qquad N_{vol}(1, m) = (m+1)(2m^2+7m+7)+1$ (A.20a)

$$= M(2M^2+3M+2)+1 \qquad M = m+1 \text{ odd}$$

$$N_{vol}(1, m) = (m+1)(2m^2+7m+7)$$ (A.20b)

$$= M(2M^2+3M+2) \qquad M = m+1 \text{ even}$$

The number of atoms on the outermost facets of an sc(*n*, *m*) NP (forming the outer polyhedral shell confining the NP) are given by the **facet count** denoted $N_{shell}(n, m)$ where simple algebra yields for

- **m even** (*N*, *M* both even or both odd)

$$N_{shell}(n, m) = 6(m+n)^2 + 2 = 6M^2 + 2$$ (A.21a)

- **m odd** (*N* even, *M* odd or *N* odd, *M* even)

$$N_{shell}(n, m) = 6(m+n)^2 = 6M^2$$ (A.21b)

with **special cases**

Generic cubic $\qquad N_{shell}(n, 0) = 6n^2 + 2 = 6N^2 + 2 \qquad N = n$ (A.22)

Generic rhombic A $\qquad N_{shell}(0, m) = 6m^2 + 2 = 6M^2 + 2 \qquad M = m \text{ even}$ (A.23a)

$$N_{shell}(0, m) = 6m^2 = 6M^2 \qquad M = m \text{ odd}$$ (A.23b)

Generic rhombic B $\qquad N_{shell}(1, m) = 6(m+1)^2 + 2 = 6M^2 + 2 \quad M = m+1 \text{ odd}$ (A.24a)

$$N_{shell}(1, m) = 6(m+1)^2 = 6M^2 \qquad M = m+1 \text{ even}$$ (A.24b)

The distances between the center of an sc(n, m) NP and its outer facet midpoints (**facet distances**) are given by $R_{\{hkl\}}(n, m)$, $\{h\,k\,l\} = \{1\,0\,0\}$, $\{1\,1\,0\}$, and $\{1\,1\,1\}$, which are connected with the polyhedral NP diameters $D_{\{hkl\}}$ according to

$$R_{\{hkl\}}(n,m) = \frac{1}{2}D_{\{hkl\}} \tag{A.25}$$

Thus, with (A.2), (A.3), (A.6), (A.7), (A.13) and a denoting the lattice constant of the sc lattice we obtain

$$R_{\{100\}}(n,m) = \frac{1}{2}N\,d_{\{100\}} = \frac{a}{2}(n+2m) \tag{A.26}$$

$$R_{\{110\}}(n,m) = \frac{1}{2}(2M)d_{\{110\}} = \frac{a}{\sqrt{2}}(n+m) \tag{A.27}$$

$$R_{\{111\}}(n,m) = \frac{1}{2}(3M)d_{\{111\}} = \frac{\sqrt{3}}{2}a(n+m) \qquad\qquad m \text{ even}^{\,+} \tag{A.28a}$$

$$= \frac{1}{2}(3M-1)d_{\{111\}} = \frac{\sqrt{3}}{2}a\left(n+m-\frac{1}{3}\right) \qquad m \text{ odd} \tag{A.28b}$$

$^{+}$ Note that for even m all $\{1\,1\,1\}$ facets reduce to one atom. Thus, distances $R_{\{111\}}(n, m)$ refer to corner rather than facet distances.

The distances between the center of an sc(n, m) NP and its two different types of corners (**corner distances**) are given by $R_{c1}(n, m)$ (referring to each of six ($n = 0$) or 24 ($n > 0$) corners at $\{1\,0\,0\}$ facets) and by $R_{c2}(n, m)$ (referring to each of eight (m even) or 24 (m odd) corners at $\{1\,1\,0\}$ (and eight possible $\{1\,1\,1\}$) facets for odd m) where with (A.7) and a denoting the lattice constant of the sc lattice

$$R_{c1}(n,m) = \frac{a}{2}\sqrt{(n+2m)^2 + 2n^2} = \frac{a}{2}\sqrt{N^2 + 2(2M-N)^2} \tag{A.29}$$

$$R_{c2}(n,m) = \frac{\sqrt{3}}{2}a(n+m) = \frac{\sqrt{3}}{2}aM \qquad\qquad m \text{ even} \tag{A.30a}$$

$$= \frac{a}{2}\sqrt{2(n+m-1)^2 + (n+m+1)^2} = \frac{a}{2}\sqrt{3(M-1)^2 + 4M} \qquad m \text{ odd} \tag{A.30b}$$

The areas of each of the $\{1\,0\,0\}$, $\{1\,1\,0\}$, and $\{1\,1\,1\}$ facets of an sc(n, m) NP, measured by corresponding corner atoms (**facet areas**), are given by $A_{\{100\}}(n, m)$ (referring to each of six facets), $A_{\{110\}}(n, m)$ (referring to each of twelve facets), and $A_{\{111\}}(n, m)$ (referring to each of six microfacets, for odd m only) where, with (A.6), (A.7) and a denoting the lattice constant of the sc lattice

$$A_{\{100\}}(n,m) = a^2 n^2 = a^2 \left(2M - N\right)^2 \tag{A.31}$$

$$A_{\{110\}}(n,m) = \frac{1}{\sqrt{2}} a^2 m \left(2n + m\right)$$

$$= \frac{1}{\sqrt{2}} a^2 \left(N - M\right)\left(3M - N\right) \qquad m \text{ even} \tag{A.32a}$$

$$A_{\{110\}}(n,m) = \frac{1}{\sqrt{2}} a^2 \left[m\left(2n + m\right) - 1 \right]$$

$$= \frac{1}{\sqrt{2}} a^2 \left[\left(N - M\right)\left(3M - N\right) - 1 \right] \qquad m \text{ odd} \tag{A.32b}$$

$$A_{\{111\}}(n,m) = \frac{\sqrt{3}}{2} a^2 \tag{A33}$$

B. Nanoparticles with Body Centered Cubic (bcc) Lattice Structure

The body centered cubic (bcc) lattice can be defined as a non-primitive simple cubic lattice by lattice vectors $\underline{R}_1$, $\underline{R}_2$, $\underline{R}_3$ in Cartesian coordinates together with two lattice basis vectors $\underline{r}_1$, $\underline{r}_2$ according to

$$\underline{R}_1 = a(1,0,0) \ , \quad \underline{R}_2 = a(0,1,0) \ , \quad \underline{R}_3 = a(0,1,0) \tag{B.1a}$$

$$\underline{r}_1 = a(0,\,0,\,0) \ , \quad \underline{r}_2 = \frac{a}{2}(1,\,1,\,1) \tag{B.1b}$$

where a is the lattice constant. The two densest monolayer families of the bcc lattice are described by six square shaped $\{1\,0\,0\}$, twelve rectangular $\{1\,1\,0\}$ (highest density), and eight hexagonal $\{1\,1\,1\}$ netplanes where distances between adjacent parallel netplanes are given by

$$d_{\{100\}} = a/2 \ , \quad d_{\{110\}} = a/\sqrt{2} \ , \quad d_{\{111\}} = a/(2\sqrt{3}) \tag{B.2}$$

The point symmetry of the bcc lattice is characterized by O_h with symmetry centers at all atom sites.

Compact body centered cubic nanoparticles (NPs) are confined by finite sections of monolayers (facets) whose structure is described by different netplanes $(h\,k\,l)$. If they exhibit central O_h symmetry and show an $(h\,k\,l)$ oriented facet they must must also include all other symmetry related facets characterized by orientations of the complete $\{h\,k\,l\}$ family. Thus, general bcc NPs of O_h symmetry are determined by facets whose orientation can be defined by those of different $\{h\,k\,l\}$ families. (As an example, we mention the $\{1\,0\,0\}$ family with its six netplane orientations $(\pm 1\,0\,0)$, $(0\,\pm 1\,0)$, $(0\,0\,\pm 1)$.) Further, according to the symmetry of the bcc host lattice possible NP centers can only be atom sites of the lattice. This will be discussed at different levels of complication in the following.

B.1. Generic bcc Nanoparticles

First, we consider generic bcc nanoparticles (NPs) of O_h symmetry which are confined by facets with orientations of only one netplane family $\{h\,k\,l\}$. This allows to distinguish between different generic NP types where we focus on those described by $\{1\,0\,0\}$ or $\{1\,1\,0\}$ facets which correspond to the densest monolayers of the bcc lattice and offer the flattest NP facets. The bcc NPs contain always an **atom** at their symmetry center.

(a) **Generic cubic** bcc NPs, denoted **bcc[N, 0)** (the notation of bcc NPs, in particular the bracketing, will be explained in Secs. B.2, 3), are confined by all six $\{1\,0\,0\}$ monolayers with distances $D_{\{100\}} = 2N\,d_{\{100\}}$ between parallel monolayers (polyhedral NP diameters).

This yields six square shaped {1 0 0} facets with $(N + 1)$ edge atoms each and eight polyhedral atom corners, see Fig. B.1.
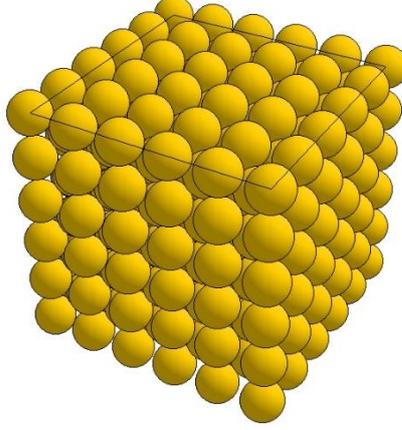
Figure B.1. Atom ball model of a generic cubic bcc NP, bcc[5, 0) with an atom at its center. The black lines sketch the square {1 0 0} facet shapes.

(b) **Generic rhombic** bcc NPs, denoted **bcc(0, M]**, are confined by all twelve {1 1 0} monolayers with distances $D_{\{110\}} = 2M\, d_{\{110\}}$ between parallel monolayers (polyhedral NP diameters). This yields rhombic {1 1 0} facets of all twelve monolayers, see Fig. B.2. The {1 1 0} rhombi contain $(M + 1) \times (M + 1)$ atoms each, also described by $2M + 1$ parallel nearest neighbor atom rows of increasing/decreasing length in the sequence 0 (atom), $1a$, …, $M\,a$, …, $1a$, 0 (atom). Altogether, the generic rhombic bcc NPs are described as rhombic dodecahedra offering 14 polyhedral atom corners and reminding of the shape of Wigner-Seitz cells of the face centered cubic (fcc) crystal lattice [a12].
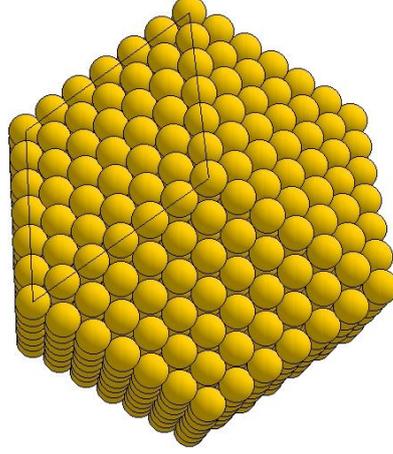
Figure B.2. Atom ball model of a generic cubic bcc(0, 6] NP with an atom at its center. The black lines sketch the rhombic {1 1 0}facet shapes.

B.2. Non-generic bcc Nanoparticles

Non-generic bcc nanoparticles of O_h symmetry are confined by facets with orientations of several netplane families $\{h_i\,k_i\,l_i\}$. This can be considered as combining the confinements of the corresponding generic NPs, NP_i, determined by $\{h_i\,k_i\,l_i\}$ with suitable polyhedral diameters, sharing their symmetry center and type (atom or void). As an example we discuss non-generic bcc nanoparticles which combine two generic nanoparticles NP_1, NP_2 of the types detailed in Sec. B.1. Thus, the resulting bcc NP contains only atoms inside both partner NPs. Here three possible scenarios can be distinguished, nanoparticle NP_2 contains all atoms of NP_1 (yielding generic NP_1), NP_1 contains all atoms of NP_2 (yielding generic NP_2), or NP_1 and NP_2 share only parts of their atoms (intersecting, which yields true non-generic NPs). These scenarios are determined by the choice of the two netplane families $\{h\,k\,l\}$ and by relationships between the corresponding polyhedral NP diameters $D_{\{hkl\}}$ defined by N and M. In the following, we restrict ourselves to non-generic sc NPs defined by pairs of generic cubic and rhombic NPs.

Non-generic bcc NPs contain always an **atom** at their symmetry center. They combine a generic cubic NP, sc[N, 0), and a rhombic NP, sc(0, M] where polyhedral diameters amount to

$$D_{\{100\}} = 2N\,d_{\{100\}} = N\,a, \qquad\qquad D_{\{110\}} = 2M\,d_{\{110\}} = 2M\,a/\sqrt{2} \qquad\qquad (B.3)$$

Thus, the smallest rhombic NP which surrounds the cubic NP is defined with (B.2) by

$$D_{\{110\}} = \sqrt{2}\,D_{\{100\}} \quad\text{and hence}\quad M = N \qquad\qquad (B.4)$$

On the other hand, the smallest cubic NP which surrounds the rhombic NP is defined with (B.2) by

$$D_{\{100\}} = \sqrt{2}\, D_{\{110\}} \quad \text{and hence} \quad N = 2M \tag{B.5}$$

As a consequence, non-generic bcc NPs combining generic cubic and rhombic NPs, NP_1, NP_2, yield the choices shown in Table B.1.

NP_1 / NP_2	NP_1 in NP_2	NP_2 in NP_1
Cubic / Rhombic bcc[N, 0) / bcc(0, M]	$M \geq N$	$N \geq 2M$

Table B.1. Constraints of structure parameters N, M for pairs of bcc NPs, NP_1 and NP_2, sharing an atom as their symmetry center.

Table B.1 shows in particular that true non-generic bcc NPs, defined by pairs of generic cubic and rhombic NPs, bcc[N, 0) and bcc(0, M] refer to structure parameters N, M which bracket each other according to

$$M < N < 2M \ , \quad N/2 < M < N \tag{B.6}$$

These non-generic bcc NPs may be called **cubo-rhombic** and denoted as **bcc[N, M]** combining a generic cubic bcc[N, 0) (first index) with a rhombic NP sc(0, M] (second index). The nomenclature together with the results of Table B.1 suggests an alternative notation for generic NPs where we may formally write

generic cubic	bcc[N, 0) = bcc[N, M] ,	$N \leq M$	(B.7a)
generic rhombic	bcc(0, M] = bcc[N, M] ,	$N \geq 2M$	(B.7b)

B.3. Cubo-rhombic bcc Nanoparticles

In the following we will discuss the detailed structure of true cubo-rhombic NPs bcc[N, M] determined by corresponding structure parameters N, M and confined by the two densest monolayer families {1 0 0} and {1 1 0}. These NPs contain always an **atom** at there symmetry center.

Starting from a generic cubic NP bcc[N, 0) with a polyhedral NP diameter $D_{\{100\}} = 2N\, d_{\{100\}}$ the smallest enclosing rhombic NP bcc(0, M] has a polyhedral NP diameter $D_{\{110\}} = 2M\, d_{\{110\}}$ with $M = N$ according to Table B.1. Shrinking the rhombic bcc NP, i.e. for smaller M values given by $M = N - m$, $m \geq 0$, the cubic and rhombic bcc NPs intersect yielding a **cubo-rhombic** NP bcc[N, $M = N - m$]. In the following we define this NP by **sc[N, m)** which is compatible with the

initial definition of a generic cubic bcc NP denoted sc[N, 0) in Sec. B.1. The constraints on M given in Table B.1 can be expressed by equivalent constraints on m yielding

$$N/2 \leq M \leq N \ , \qquad 0 \leq m \leq N/2 \tag{B.8}$$

where m values larger than $N/2$ result in generic rhombic bcc NPs. The building scheme corresponds to the generic cubic NP bcc[N, 0) being truncated at its twelve edges by removing m {1 1 0} facet layers each.

On the other hand, starting from a generic rhombic NP, bcc(0, M], with a polyhedral NP diameter $D_{\{110\}} = 2M\, d_{\{110\}}$ the smallest enclosing cubic bcc NP has a polyhedral NP diameter $D_{\{100\}} = 2N\, d_{\{100\}}$ with $N = 2M$ according to Table B.1. Shrinking the cubic bcc NP, i.e. for smaller N values given by $N = 2M$ - n with $n \geq 0$, the cubic and rhombic NPs intersect yielding also a **cubo-rhombic** NP bcc[$N = 2M$ - n, M]. In the following we define this NP by **bcc(n, M]** which is compatible with the initial definition of a generic rhombic bcc NP denoted bcc(0, M] in Sec. A.1. The constraints on N given in Table B.1 can be expressed by equivalent constraints on n yielding

$$M \leq N \leq 2M \ , \qquad 0 \leq n \leq M \qquad \text{cubo-rhombic A (\textit{N} even)} \tag{B.9}$$

where n values larger than M result in generic cubic bcc NPs. The building scheme corresponds to the generic rhombic NP, sc(0, M], being truncated at its six 4-fold symmetry corners by removing n {1 0 0} facet layers each.

The two building schemes must yield the same cubo-rhombic NP bcc[N, M] where the two structure parameters N, M quantify the polyhedral NP diameters $D_{\{100\}}$ and $D_{\{110\}}$ according to

$$D_{\{100\}} = 2N\, d_{\{100\}} \ , \qquad D_{\{110\}} = 2M\, d_{\{110\}} \tag{B.10}$$

with the basic netplane distances $d_{\{100\}}$ and $d_{\{110\}}$ given by (B.2). Further, the relations

$$M = N - m \ , \qquad N = 2M - n \tag{B.11a}$$

from the two building schemes can be converted to

$$n = 2M - N \ , \qquad m = N - M \tag{B.11b}$$

$$N = n + 2m \ , \qquad M = n + m \tag{B.11c}$$

This suggest an alternative set of structure parameters n, m which characterize the deviation of the cubo-rhombic NP bcc[N, M] from its generic envelope NPs, cubic bcc[N, 0) and rhombic bcc(0, M]. Thus, **cubo-rhombic** bcc NPs can also be denoted **bcc(n, m)**.

The structure parameters n, m are also connected with geometric properties of the NP facets, in particular, with characteristic lengths of the facet edges. The cubo-rhombic bcc NPs, bcc[N, M] $\equiv$ bcc(n, m), are confined by all six {1 0 0} facets of square shape with $(n + 1) \times (n + 1)$ atoms each and by all twelve {1 1 0} facets, see Fig. B.3. The {1 1 0} facets are hexagonal and contain $2m + 1$ parallel nearest neighbor atom rows of increasing/decreasing length in the sequence $n\,a$, $(n+1)a$, …, $(n + m)a$, …, $(n+1)a$, $n\,a$. Altogether, the bcc NPs are described by cubo-rhombic polyhedra offering 32 ($n > 0$, $m > 0$) corners with true cubic ($n > 0$, $m = 0$, eight corners) and true rhombic ($n = 0$, $m > 0$, 14 corners) being special cases.
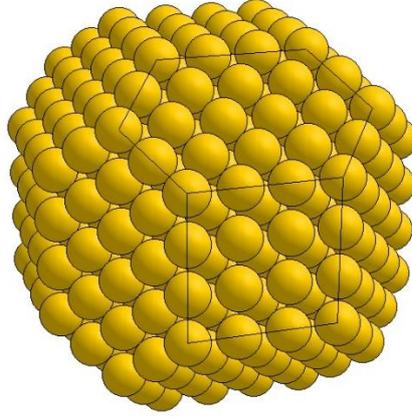
Figure B.3. Atom ball model of the cubo-rhombic sc[7, 5] $\equiv$ bcc(3, 2) NP. The black lines sketch the square {1 0 0} and hexagonal {1 1 0} facet shapes.

The confinement of a cubo-rhombic bcc[N, M] $\equiv$ bcc(n, m) NP by its generic envelope bcc NPs, cubic bcc[N, 0) and rhombic bcc(0, M] with N, M defined by B.11, is illustrated in Fig. B.4 for bcc[10, 7] $\equiv$ bcc(4, 3) with bcc[10, 0) and bcc(0, 7] forming the envelope bcc NPs.

(a) (b) (c)
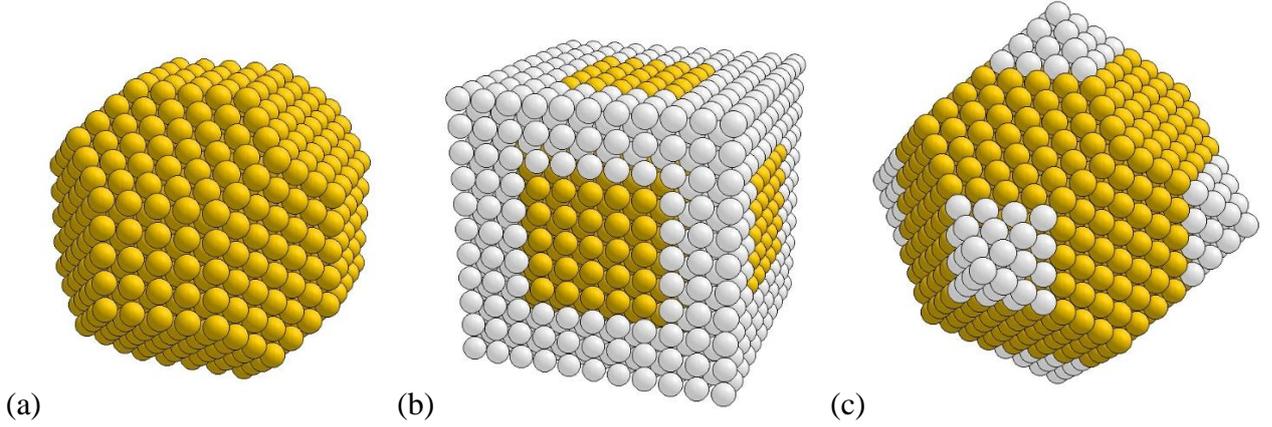
Figure B.4. Atom ball models of a cubo-rhombic bcc[10, 7] ≡ bcc(4, 3) NP with its confining generic cubic and rhombic NPs. (a) Initial bcc(4, 3) shown by yellow balls, (b) bcc(4, 3) inside generic bcc[10, 0), and (c) bcc(4, 3) inside generic bcc(0, 7]. The atoms outside bcc(4, 3) are shown by white balls.

Altogether, the equivalence of structure parameters n, m and N, M according to (B.11) suggests alternative notations of cubo-rhombic bcc NPs introduced earlier. Apart from a notation by bcc[N, M], meaningful alternatives are bcc(n, m), bcc[N, m), and bcc(n, M] where the different bracketing denotes the different meanings of the two parameters in the notation. Table B.2 lists types and notations of all intersecting cubo-rhombic bcc NPs.

Type	bcc(n, m)	bcc[N, M]	bcc[N, m)	bcc(n, M]
Cubo-rhombic	$n > 0, m > 0$	$M < N < 2M$	$0 < m < N/2$	$0 < n < M$
Generic cubic	$n > 0, m = 0$	$N = M$	$m = 0$	$n = M$
Generic rhombic	$n = 0, m > 0$	$N = 2M$	$m = N/2$	$n = 0$
Atom (A)	$n = m = 0$	$N = M = 0$	$N = m = 0$	$n = M = 0$

Table B.2. Types and notations of all intersecting and generic bcc NPs.

B.4. Properties of Cubo-rhombic bcc Nanoparticles

Structural properties characterizing cubo-rhombic bcc nanoparticles can be obtained by geometric consideration and simple algebra where we quote only results of the most important quantities. Structure parameters n, m and N, M, according to (B.11), i.e.

$$n = 2M - N \ , \qquad\qquad m = N - M \qquad\qquad\qquad (\text{B.11b})$$

$$N = n + 2m \ , \qquad\qquad M = n + m \qquad\qquad\qquad (\text{B.11c})$$

with constraints listed in Table B.1 will be used interchangeably and in mixed combinations to simplify formal expressions. Note that according to (B.11) structure parameters n and N will always be both even or both odd numbers.

The number of atoms forming a bcc(n, m) NP are given by the **volume count** denoted $N_{vol}(n, m)$ where simple algebra yields

$$
\begin{aligned}
N_{vol}(n,\ m) &= \frac{1}{2}(2n+2m+1)\left[(2n+2m+1)^2+1\right]-n(n+1)(2n+1) \\
&= \frac{1}{2}(2M+1)\left[(2M+1)^2+1\right]-n(n+1)(2n+1)
\end{aligned}
\qquad (\text{B.12})
$$

with **special cases**

Generic cubic
$$
\begin{aligned}
N_{vol}(n,\ 0) &= (2n+1)\left[n(n+1)+1\right] \\
&= (4M-2N+1)\left[(2M-N)(2M-N+1)+1\right] \quad (\text{B.13})
\end{aligned}
$$

Generic rhombic
$$
\begin{aligned}
N_{vol}(0,\ m) &= (2m+1)\left[2m(m+1)+1\right] \\
&= (2(N-M)+1)\left[2(N-M)(N-M+1)+1\right] \quad (\text{B.14})
\end{aligned}
$$

The number of atoms on the outermost facets of a bcc(n, m) NP (forming the outer polyhedral shell confining the NP) are given by the **facet count** denoted $N_{shell}(n, m)$ where simple algebra yields

$$N_{shell}(n,m) = 12(n+m)^2 - 6n^2 + 2 = 12M^2 - 6(2M-N)^2 + 2 \qquad (\text{B.15})$$

with **special cases**

Generic cubic
$$
\begin{aligned}
N_{shell}(n,0) &= 6n^2 + 2 \\
&= 6(2M-N)^2 + 2 \qquad n>0 \qquad (\text{B.16})
\end{aligned}
$$

Generic rhombic
$$
\begin{aligned}
N_{shell}(0,m) &= 12m^2 + 2 \\
&= 12(N-M)^2 + 2 \qquad m>0 \qquad (\text{B.17})
\end{aligned}
$$

The distances between the center of a bcc(n, m) NP and its outer facet midpoints (**facet distances**) are given by $R_{\{hkl\}}(\boldsymbol{n}, \boldsymbol{m})$, $\{h\,k\,l\} = \{1\,0\,0\}$, $\{1\,1\,0\}$, and $\{1\,1\,1\}$, which are connected with the polyhedral NP diameters $D_{\{hkl\}}$ according to

$$R_{\{hkl\}}(n,m) = \frac{1}{2} D_{\{hkl\}} \tag{B.18}$$

Thus, with (B.2), (B.3), (B.11) and a denoting the lattice constant of the bcc lattice we obtain

$$R_{\{100\}}(n,m) = \frac{1}{2}(2N)d_{\{100\}} = \frac{a}{2}(n+2m) \tag{B.19}$$

$$R_{\{110\}}(n,m) = \frac{1}{2}(2M)d_{\{110\}} = \frac{a}{\sqrt{2}}(n+m) \tag{B.20}$$

$$R_{\{111\}}(n,m) = \frac{1}{2}(6M)d_{\{111\}} = \frac{\sqrt{3}}{2}a(n+m) \tag{B.21}$$

[+] Note that all $\{1\,1\,1\}$ facets reduce to one atom. Thus, distances $R_{\{111\}}(\boldsymbol{n}, \boldsymbol{m})$ refer to corner rather than facet distances.

The distances between the center of a bcc(n, m) NP and its two different types of corners (**corner distances**) are given by $R_{c1}(\boldsymbol{n}, \boldsymbol{m})$ (referring to each of six ($n = 0$) or 24 ($n > 0$) corners at $\{1\,0\,0\}$ facets) and by $R_{c2}(\boldsymbol{n}, \boldsymbol{m})$ (referring to each of eight corners at $\{1\,1\,0\}$)) where, with (B.11) and a denoting the lattice constant of the bcc lattice

$$R_{c1}(n,m) = \frac{a}{2}\sqrt{(n+2m)^2 + 2n^2} = \frac{a}{2}\sqrt{N^2 + 2(2M-N)^2} \tag{B.22}$$

$$R_{c2}(n,m) = \frac{\sqrt{3}}{2}a(n+m) = \frac{\sqrt{3}}{2}aM = R_{\{111\}}(n,m) \tag{B.23}$$

The areas of each of the $\{1\,0\,0\}$ and $\{1\,1\,0\}$ facets of a bcc(n, m) NP, measured by corresponding corner atoms (**facet areas**), are given by $A_{\{100\}}(\boldsymbol{n}, \boldsymbol{m})$ (referring to each of six facets) and $A_{\{110\}}(\boldsymbol{n}, \boldsymbol{m})$ (referring to each of twelve facets) where, with a denoting the lattice constant of the bcc lattice

$$A_{\{100\}}(n,m) = a^2 n^2 = a^2(2M-N)^2 \tag{B.24}$$

$$A_{\{110\}}(n,m) = \frac{1}{\sqrt{2}}a^2 m(2n+m) = \frac{1}{\sqrt{2}}a^2(N-M)(3M-N) \tag{B.25}$$

C. Nanoparticles with Face Centered Cubic (fcc) Lattice Structure

The face centered cubic (fcc) lattice can be defined as a non-primitive simple cubic lattice by lattice vectors $\underline{R}_1$, $\underline{R}_2$, $\underline{R}_3$ in Cartesian coordinates together with four lattice basis vectors $\underline{r}_1$ to $\underline{r}_4$ according to

$$\underline{R}_1 = a(1,0,0) \,, \quad \underline{R}_2 = a(0,1,0) \,, \quad \underline{R}_3 = a(0,1,0) \tag{C.1a}$$

$$\underline{r}_1 = a(0,0,0) \,, \quad \underline{r}_2 = a/2\,(0,1,1) \,, \quad \underline{r}_3 = a/2\,(1,0,1) \,, \quad \underline{r}_4 = a/2\,(1,1,0) \tag{C.1b}$$

where a is the lattice constant. The two densest monolayer families of the fcc lattice are described by six square shaped {1 0 0} and eight hexagonal {1 1 1} (highest density) netplanes where distances between adjacent parallel netplanes are given by

$$d_{\{100\}} = a/2 \,, \quad d_{\{111\}} = a/\sqrt{3} \,, \quad d_{\{110\}} = a/(2\sqrt{2}) \tag{C.2}$$

The point symmetry of the fcc lattice is characterized by O_h with symmetry centers at all atom sites and at the void centers of each elementary cell.

Compact face centered cubic nanoparticles (NPs) are confined by finite sections of monolayers (facets) whose structure is described by different netplanes $(h\,k\,l)$. If they exhibit central O_h symmetry and show an $(h\,k\,l)$ oriented facet they must must also include all other symmetry related facets characterized by orientations of the complete $\{h\,k\,l\}$ family. Thus, general fcc NPs of O_h symmetry are determined by facets whose orientation can be defined by those of different $\{h\,k\,l\}$ families. (As an example, we mention the {1 1 1} family with its eight netplane orientations $(\pm1\,\pm1\,\pm1)$.) Further, according to the symmetry of the fcc host lattice possible NP centers can only be atom or O_h symmetry void sites of the lattice. This will be discussed at different levels of complication in the following.

C.1. Generic fcc Nanoparticles

First, we consider generic fcc nanoparticles (NPs) of O_h symmetry which are confined by facets with orientations of only one netplane family $\{h\,k\,l\}$. This allows to distinguish between different generic NP types where we focus on those confined by {1 0 0} or {1 1 1} facets which correspond to the densest monolayers of the fcc lattice and offer the flattest NP facets.

(a)   **Generic cubic** fcc NPs are confined by all six {1 0 0} monolayers with distances $D_{\{100\}} = 2N \, d_{\{100\}}$ between parallel monolayers (polyhedral NP diameters). Here we distinguish two NP types.

Generic cubic A fcc NPs, denoted **fcc[N, 0)** (the notation of fcc NPs, in particular the bracketing, will be explained in Secs. C.2, 3) contain an **atom** at their symmetry center for **even** N and a **void** for **odd** N. They are confined by true square {1 0 0} facets. This yields facets with $(N + 1)$ edge atoms each and eight polyhedral atom corners, see Fig. C.1a.

Generic cubic B fcc NPs, denoted **fcc[N, 1)** contain an **atom** at their symmetry center for **odd** N and a **void** for **even** N. They are confined by capped square (octagonal) {1 0 0} facets with long edges of N atoms each and eight polyhedral atom corners capped by {1 1 1} microfacets, see Fig. C.1b. .

(a)   (b)
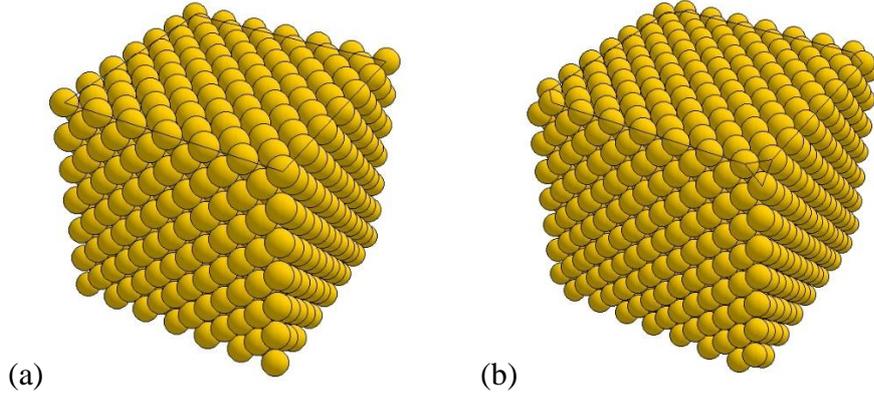
Figure C.1. Atom ball models of generic cubic fcc NPs, (a) cubic A fcc[6, 0) and (b) cubic B fcc[7, 1). The black lines sketch the square and octagonal {1 0 0} as well as the triangular {1 1 1} facet shapes.

(b)   **Generic octahedral** fcc NPs are confined by all eight {1 1 1} monolayers with distances $D_{\{111\}} = K \, d_{\{111\}}$ between parallel monolayers (polyhedral NP diameters). These NPs contain an **atom** at their symmetry center for **even** K and a void **void** for **odd** K. Here we distinguish two NP types.

Generic octahedral A fcc NPs, denoted **fcc(0, K]**, are confined by true triagonal facets with $(K + 1)$ edge atoms each six polyhedral atom corners, see Fig. C.2a.

Generic octahedral B fcc NPs, denoted **fcc(1, K]**, are confined by capped triagonal (hexagonal) {1 1 1} facets with long edges of N - 1 atoms each and six capped polyhedral atom corners with {1 0 0} microfacets. These NPs are not strictly generic since they are

derived from generic octahedral A, fcc(0, *K*] , by removing all six corner atoms. How-
ever, they will be useful in the discussion of Sec. C.2 and later.

(a)   (b)
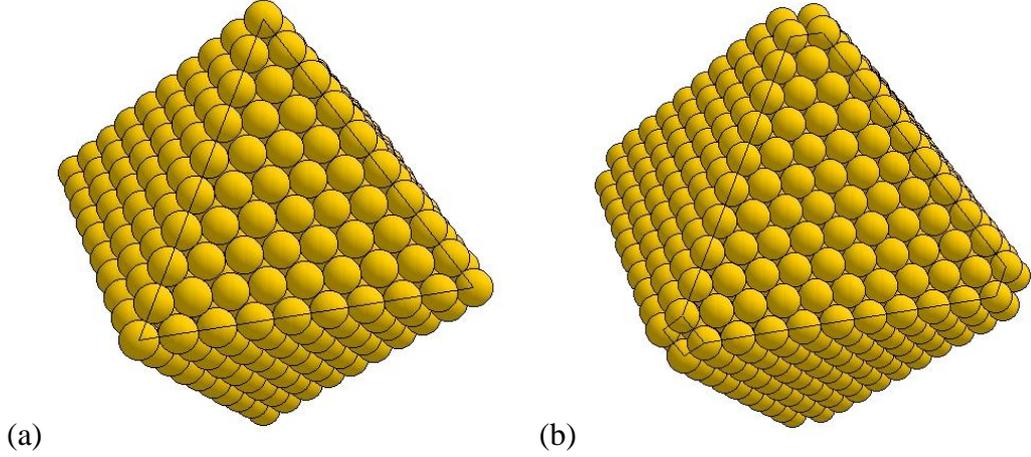
Figure C.2. Atom ball models of generic octahedral fcc NPs, (a) octahe-
dral A fcc(0, 9] and (b) octahedral B fcc(1, 11] . The black lines sketch
the triangular {1 1 1} and square {1 0 0}facet shapes.

(c)   **Generic cuboctahedral** fcc NPs, denoted **fcc(*N*, 2*N*]** (the notation, in particular the
bracketing, will be explained in Secs. C.2, 3), contain always an **atom** at their symmetry
center. They are confined by the six {1 0 0} monolayers with distances $D_{\{100\}} = 2N\, d_{\{100\}}$
as well as by the eight {1 1 1} monolayers with distances $D_{\{111\}} = 2N\, d_{\{111\}}$ between par-
allel monolayers (polyhedral NP diameters). They are described by six square shaped
{1 0 0} facets with $(N + 1) \times (N + 1)$ atoms each and by eight triangular shaped {1 1 1}
facets with $(n + 1)$ atom edges, see Fig. C.3b.
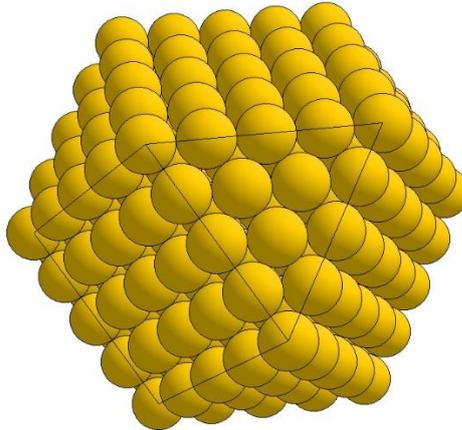
Figure C.3. Atom ball model of a generic cuboctahedral NP fcc(4, 8].
The black lines sketch the square {1 0 0} and triangular {1 1 1} facet
shapes.

C.2. Non-generic fcc Nanoparticles

Non-generic fcc nanoparticles of O_h symmetry are confined by facets with orientations of several netplane families $\{h_i\ k_i\ l_i\}$. This can be considered as combining the confinements of the corresponding generic NPs, NP_i, determined by $\{h_i\ k_i\ l_i\}$ with suitable polyhedral diameters, sharing their symmetry center and type (atom or void). As an example we discuss non-generic fcc nanoparticles which combine two generic nanoparticles NP_1, NP_2 of the types detailed in Sec. C.1. Thus, the resulting fcc NP contains only atoms inside both partner NPs. Here three possible scenarios can be distinguished, nanoparticle NP_2 contains all atoms of NP_1 (yielding generic NP_1), NP_1 contains all atoms of NP_2 (yielding generic NP_2), or NP_1 and NP_2 share only parts of their atoms (intersecting which yields true non-generic NPs). These scenarios are determined by the choice of the two netplane families $\{h\ k\ l\}$ and by relationships between the corresponding polyhedral NP diameters $D_{\{hkl\}}$ defined by N and K. In the following, we restrict ourselves to non-generic fcc NPs defined by pairs of generic cubic and octahedral NPs.

Non-generic fcc NPs with an **atom** at their symmetry center combine a generic cubic NP (cubic A, fcc[N, 0) with even N, or cubic B, fcc[N, 1) with odd N), with a generic octahedral NP (octahedral A, B, fcc(0, K], fcc(1, K] with even K) where polyhedral diameters amount to

$$D_{\{100\}} = 2N\, d_{\{100\}} = N\, a, \quad D_{\{111\}} = K\, d_{\{111\}} = K\, a/\sqrt{3} \tag{C.3}$$

Thus, the smallest octahedral NP which surrounds a cubic A or B NP is defined with (C.2) by

cubic A: $\quad D_{\{111\}} = \sqrt{3}\, D_{\{100\}}$ $\qquad$ and hence $\quad K = 3N$ $\qquad$ (C.4a)

cubic B: $\quad D_{\{111\}} = \sqrt{3}\, D_{\{100\}} - 2d_{\{111\}}/2$ $\quad$ and hence $\quad K = 3N - 1$ $\qquad$ (C.4b)

On the other hand, the smallest cubic NP surrounding an octahedral A, B NP is defined with (C.2) by

octahedral A: $D_{\{100\}} = \sqrt{3}\, D_{\{111\}}$ $\qquad$ and hence $\quad N = K$ $\qquad$ (C.5a)

octahedral B: $D_{\{100\}} = \sqrt{3}\, D_{\{111\}} - 2d_{\{100\}}$ $\quad$ and hence $\quad N = K - 1$ $\qquad$ (C.5b)

As a consequence, non-generic fcc NPs with an atom at their symmetry center combining generic cubic and rhombic NPs, NP_1 / NP_2, yield the three choices shown in Table C.1.

NP$_1$ / NP$_2$	NP$_1$ in NP$_2$	NP$_2$ in NP$_1$
Cubic A / Octahedral A fcc[N, 0) / fcc(0, K]	$K \geq 3N$	$N \geq K$
Cubic B / Octahedral B fcc[N, 1) / fcc(1, K]	$K \geq 3N - 1$	$N \geq K - 1$
Cubic A / Octahedral B fcc[N, 0) / fcc(1, K]	$K \geq 3N$	$N \geq K$ (<)
Cubic B / Octahedral A fcc[N, 1) / fcc(0, K]	$K \geq 3N - 1$	$N \geq K + 1$ (<)

Table C.1. Constraints of structure parameters N, M for pairs of fcc NPs, NP$_1$ and NP$_2$, sharing an atom or void as their symmetry center. Entries labeled (<) refer to combinations NP$_1$ / NP$_2$ where NP$_2$ never touches the surface of NP$_1$.

Non-generic fcc NPs with a **void** at their symmetry center combine a generic cubic NP (cubic A, C, fcc[N, 0) with odd N, or cubic B, fcc[N, 1) with even N), with a generic octahedral NP (octahedral A, B, fcc(0, K], fcc(1, K] with odd K) where, in complete analogy to the atom centered NPs, polyhedral diameters are given by (C.3). Further, smallest octahedral NPs surrounding a cubic A or B NPs are defined by (C.4) and smallest cubic NPs surrounding octahedral A, B NPs by (C.5). This shows that Table 1 applies also to NPs with a void at their symmetry center if N, K are chosed accordingly.

Table C.1 shows in particular that true non-generic fcc NPs, defined by pairs of generic cubic NPs, fcc[N, p), $p = 0$, 1, and octahedral NPs, fcc(q, K], $q = 0$, 1, refer to structure parameters N, K which bracket each other. As examples we mention

$$N < K < 3N \qquad \text{fcc}[N, 0) / \text{fcc}(0, K] \qquad (C.6a)$$

$$N + 1 < K < 3N - 1 \qquad \text{fcc}[N, 1) / \text{fcc}(1, K] \qquad (C.6c)$$

These non-generic fcc NPs may be called **cuboctahedral** and denoted as **fcc[N, M]** combining a generic cubic (first index) with an octahedral NP (second index) where cubic A NPs combine with octahedral A and cubic B with octahedral B fcc NPs.

The nomenclature together with the results of Table C.1 suggests an alternative notation for generic NPs where we may formally write

generic cubic A, B $\qquad$ fcc[N, p) = fcc[N, K] $\qquad K \geq 3N - p$, $p = 0$, 1, 2 $\quad$ (C.7a)

generic octahedral A, B $\qquad$ fcc(q, K] = fcc[N, K] $\qquad N \geq K - q$, $q = 0$, 1 $\qquad$ (C.7b)

C.3. Cuboctahedral fcc Nanoparticles

In the following we will discuss the detailed structure of true cuboctahedral NPs fcc[N, K] determined by corresponding structure parameters N, K and confined by the two densest monolayer families {1 0 0} and {1 1 1}. These NPs contain an **atom** at there symmetry center for **even K** while their symmetry center is **void** for **odd K**.

First, we consider **atom centered** fcc NPs. Starting from a generic cubic A NP fcc[N, 0) with even N and a polyhedral NP diameter $D_{\{100\}} = 2N\, d_{\{100\}}$ the smallest enclosing octahedral A NP fcc(0, K] has a polyhedral NP diameter $D_{\{111\}} = K\, d_{\{111\}}$ with even $K = 3N$ according to Table C.1. Shrinking the octahedral fcc NP, i.e. for smaller K values given by $K = 3N - k$, $k = 0, 2, 4 \ldots$ the cubic and octahedral fcc NPs intersect yielding a **cuboctahedral** NP fcc[N, $K = 3N - k$]. In the following we define this NP by **fcc[N, k)** which is compatible with the initial definition of a generic cubic fcc NP denoted fcc[N, 0) in Sec. C.1. The constraints on K given in Table C.1 can be expressed by equivalent constraints on k yielding

$$N \le K \le 3N \ , \qquad\qquad 0 \le k \le 2N \ \text{ with even } k \qquad\qquad \text{(C.8a)}$$

where k values larger than $2N$ result in generic octahedral fcc NPs.

Starting from a generic cubic B NP fcc[N, 1) with odd N and a polyhedral NP diameter $D_{\{100\}} = 2N\, d_{\{100\}}$ the smallest enclosing octahedral B NP fcc(1, K] has a polyhedral NP diameter $D_{\{111\}} = K\, d_{\{111\}}$ with even $K = 3N - 1$ according to Table C.1. Shrinking the octahedral fcc NP, i.e. for smaller K values given by $K = 3N - k$, $k = 1, 3, 5 \ldots$ the cubic and octahedral fcc NPs intersect yielding also a **cuboctahedral** NP fcc[N, $K = 3N - k$] which we define by **fcc[N, k)**. Here the constraints on K in Table C.1 lead to constraints on k according to

$$N + 1 \le K \le 3N - 1 \ , \qquad\qquad 1 \le k \le 2N - 1 \ \text{ with odd } k \qquad\qquad \text{(C.8b)}$$

where k values larger than $2N$ result in generic octahedral fcc NPs.

As a result, the two building schemes for all possible values of N correspond to generic cubic A or B NPs, fcc[N, 0) or fcc[N, 1), being truncated at their eight edges by removing $k/2$ or $(k - 1)/2$ {1 1 1} facet layers each.

On the other hand, starting from a generic octahedral A NP, fcc(0, K] with even $K = 3p$, i.e. being also a multiple of 3 (or with $K = 3p - 2$) and a polyhedral NP diameter $D_{\{111\}} = K\, d_{\{111\}}$ the smallest enclosing cubic A fcc NP fcc[N, 0) has a polyhedral NP diameter $D_{\{100\}} = 2N\, d_{\{100\}}$ with even $N = K$ according to Table C.1. Shrinking the cubic fcc NP, i.e. for smaller N values given

by $N = K - n$ with $n = 0, 2, 4 \ldots$ the cubic and octahedral NPs intersect yielding also a **cubocta-hedral** fcc[$N = K - n, K$] with even n. In the following we define this NP by **fcc(n, K]** which is compatible with the initial definition of a generic octahedral fcc NP denoted sc(0, K] in Sec. C.1. The constraints on N given in Table C.1 can be expressed by equivalent constraints on n yielding

$$K/3 \leq N \leq K \ , \qquad\qquad 0 \leq n \leq (2/3)K \ , \quad n \text{ even} \qquad\qquad \text{(C.9a)}$$

where n values larger than $(2/3)K$ result in generic cubic fcc NPs.

For an octahedral B NP fcc(1, K] with even $K = 3p - 1$ the smallest enclosing cubic NP is fcc[N, 1) and has a polyhedral NP diameter $D_{\{100\}} = 2N\,d_{\{100\}}$ with odd $N = K - 1$ according to Table C.1. Shrinking the cubic fcc NP, i.e. for $N = K - n$ with $n = 1, 3, 5 \ldots$ the cubic and octahedral NPs intersect yielding also a **cuboctahedral** fcc[$N = K - n, K$] defined as **fcc(n, K]**, however, with odd n. This leads to constraints on n, together with Table C.1

$$(K + 1)/3 \leq N \leq K - 1 \ , \qquad 1 \leq n \leq (2K - 1)/3 \ , \quad n \text{ odd} \qquad\qquad \text{(C.9b)}$$

where n values larger than $(2K - 1)/3$ result in generic cubic fcc NPs.

As a result, the building schemes for all possible values of K correspond to generic octahedral A or B NPs, fcc(0, K] or fcc(1, K], being truncated at their six 4-fold symmetry corners by removing n or $(n - 1)\{1\,0\,0\}$ facet layers each.

The two building scenarios, starting from a generic octahedral or generic cubic NPs, must yield the same cuboctahedral NP fcc[N, M] where the two structure parameters N, K quantify the poly-hedral NP diameters $D_{\{100\}}$ and $D_{\{111\}}$ according to

$$D_{\{100\}} = 2N\,d_{\{100\}} \ , \qquad\qquad D_{\{111\}} = K\,d_{\{11\}} \qquad\qquad \text{(C.10)}$$

with the basic netplane distances $d_{\{100\}}$ and $d_{\{111\}}$ given by (C.2). Further, the relations

$$N = K - n \ , \qquad\qquad K = 3N - k \ , \qquad\qquad \text{(C.11a)}$$

from the two building schemes can be converted to

$$n = K - N \ , \qquad\qquad k = 3N - K \qquad\qquad \text{(C.11b)}$$

$$2N = n + k \ , \qquad\qquad 2K = 3n + k \qquad\qquad \text{(C.11c)}$$

Next, we consider **void centered** fcc NPs whose treatment is completely analogous to the atom centered case. In fact, all derivations and relationships (C.8a) to (C.11c) are identical with those obtained for atom centered NPs except that all N or K values which are even with one centering will be odd with the other and viceversa.

Altogether, relation (C.11) suggest an alternative set of structure parameters n, k which characterize the deviation of the cuboctahedral NP fcc[N, K] from its generic envelope NPs, cubic fcc[N, 0) or fcc[N, 1) and rhombic fcc(0, K] or fcc(1, K]. Thus, **cuboctahedral** NPs can also be denoted **fcc(*n*, *k*)**.

The structure parameters n, k are also connected with geometric properties of the NP facets, in particular, with characteristic lengths of the facet edges where we can distinguish two types of cuboctahedral fcc NPs, **truncated octahedral** and **truncated cubic** species.

Truncated octahedral NPs, fcc[N, K] / fcc(n, k) with (C.11) are defined by

$$N \leq K \leq 2N , \qquad 0 \leq n \leq N , \qquad N \leq k \leq 2N , \qquad \text{i.e. } n \leq k \qquad \text{(C.12a)}$$

where the symmetry center is an atom site for even K (N, n, k all even or all odd) or void for odd K (N even and n, k odd or N odd and n, k even). These NPs are confined by all six {1 0 0} facets of square shape with $(n + 1) \times (n + 1)$ atoms each and by all eight {1 1 1} facets of hexagonal shape with alternating $(n + 1)$ and $(k - n + 2)/2$ atom edges, see Fig. C.4. The polyhedral NPs offer 24 ($n > 0$, $k > N$) corners with true octahedral ($n = 0$, $k = 2N$, six corners) and generic cuboctahedral ($n = k = N$, twelve corners) being special cases.
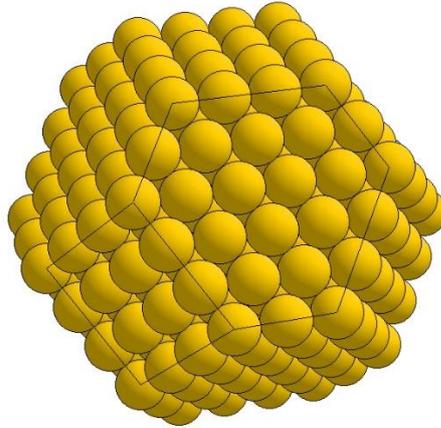
Figure C.4. Atom ball model of a truncated octahedral NP fcc[5, 8] $\equiv$ fcc(3, 7) $\equiv$ fcc(3, 2)$_\text{o}$. The black lines sketch the square {1 0 0} and hexagonal {1 1 1} facet shapes.

As a result of the building procedure, truncated octahedral fcc[N, K] NPs are each confined by two generic NPs, one octahedral fcc(0, K] or fcc(1, K] NP and one cubic fcc(N, 0) or fcc(N, 1). This is illustrated for the NP fcc[5, 8] $\equiv$ fcc(3, 2)$_\text{o}$ in Fig. C.5.
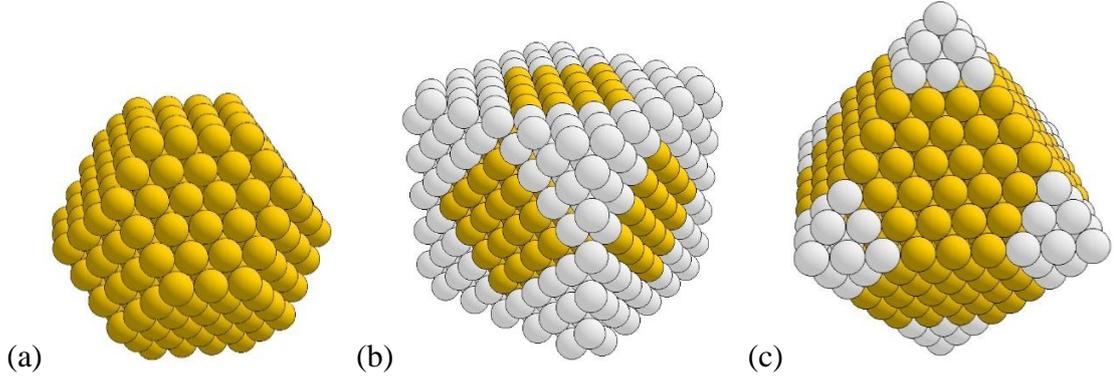
Figure C.5. Atom ball models of a truncated octahedral NP fcc[5, 8] $\equiv$ fcc(3, 2)$_o$ with its confining generic cubic and octahedral NPs. (a) Initial fcc(3, 2)$_o$ shown by yellow balls, (b) fcc(3, 2)$_o$ inside generic fcc[5, 1], and (c) fcc(3, 2)$_o$ inside generic fcc(0, 8]. The atoms outside fcc(3, 2)$_o$ are shown by white balls.

Further, Fig. C.6 shows the generic cuboctahedral NP fcc(4, 8] $\equiv$ fcc(4, 0)$_o$ with its confining generic cubic fcc[4, 0) and octahedral fcc(0, 8] NPs.
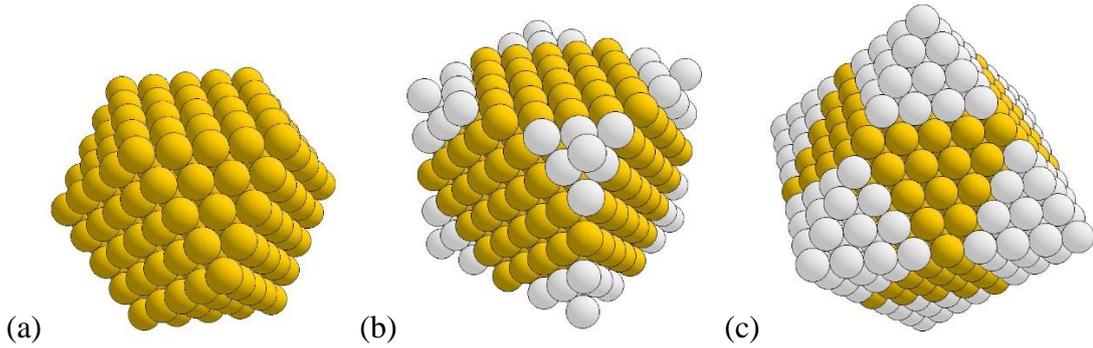
Figure C.6. Atom ball models of a cuboctahedral NP fcc[4, 8] $\equiv$ fcc(4, 0)$_o$ $\equiv$ fcc(0, 4)$_c$ with its confining generic cubic and octahedral NPs. (a) Initial fcc(4, 0)$_o$ shown by yellow balls, (b) fcc(4, 0)$_o$ inside generic fcc[4, 0), and (c) fcc(4, 0)$_o$ inside generic fcc(0, 8]. The atoms outside fcc(4, 0)$_o$ are shown by white balls.

Truncated cubic NPs, fcc[N, K] / fcc(n, k) with (C.11) are defined by

$$2N \leq K \leq 3N , \quad N \leq n \leq 2N , \quad 0 \leq k \leq N , \quad \text{i.e. } k \leq n \quad \text{(C.12b)}$$

where the symmetry center is an atom site for even K (N, n, k all even or all odd) or void for odd K (N even and n, k odd or N odd and n, k even). They are confined by all six {1 0 0} facets of octagonal shape with alternating ($n - k + 2$)/2 and ($k + 1$) atom edges and by all eight {1 1 1} facets of triangular shape with edges of $k + 1$ atoms each , see Fig. C.7. The polyhedral NPs offer 24 ($n > 0$, $k > 0$) corners with cuboctahedral ($n = 0$, $k > 0$, twelve corners) and true cubic ($n > 0$, $k = 0$, eight corners) being special cases.
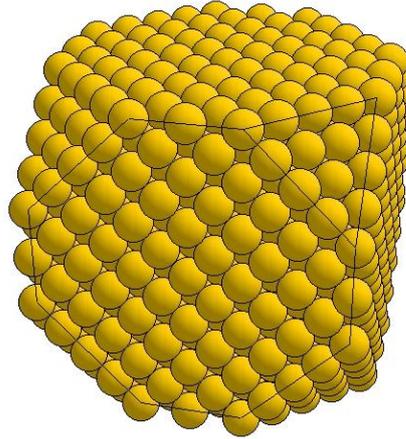
Figure C.7. Atom ball model of a truncated cubic NP, fcc[6, 14] ≡ fcc(8, 4) ≡ fcc(2, 4)$_c$. The black lines sketch the octagonal {1 0 0} and triangular {1 1 1} facet shapes.

As a result of the building procedure, truncated cubic fcc[N, K] NPs are each confined by two generic NPs, one octahedral fcc(0, K] or fcc(1, K] NP and one cubic fcc(N, 0) or fcc(N, 1). This is illustrated for the NP fcc[6, 14] ≡ fcc(2, 4)$_c$ in Fig. C.8.

(a) (b) (c)
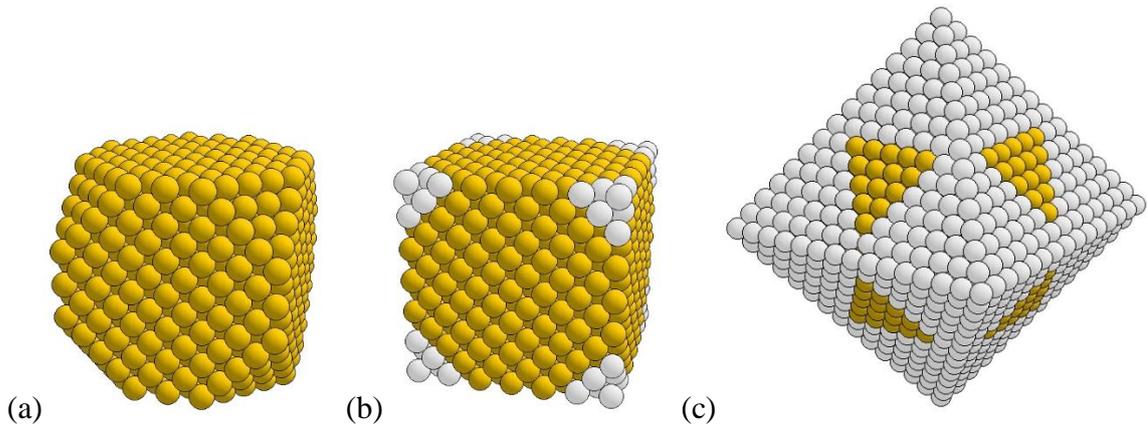
Figure C.8. Atom ball models of a cuboctahedral NP fcc[6, 14] ≡ fcc(2, 4)$_c$ with its confining generic cubic and octahedral NPs. (a) Initial fcc(2, 4)$_c$ shown by yellow balls, (b) fcc(2, 4)$_c$ inside generic fcc[6, 0], and (c) fcc(2, 4)$_c$ inside generic fcc(0, 14]. The atoms outside fcc(2, 4)$_c$ are shown by white balls.

Altogether, the equivalence of structure parameters n, k and N, K according to (C.11) suggests alternative notations of cuboctahedral fcc NPs introduced earlier. Apart from a notation by fcc[N, K], meaningful alternatives are fcc(n, k), fcc[N, k), and fcc(n, K] where the different bracketing denotes the different meanings of the two parameters in the notation. Table C.2 lists types and notations of all cuboctahedral fcc NPs where atom centered NPs refer to even K values while for void centered NPs K values are odd.

Type	fcc[N, M]	fcc(n, k)	fcc[N, k]	fcc(n, K]
Cuboctahedral, truncated octahedral	$N \leq K \leq 2N$ $n \leq k$	$0 \leq n \leq N$ $N \leq k \leq 2N$	$N \leq k \leq 2N$	$0 \leq n \leq N$
Cuboctahedral, truncated cubic	$2N \leq K \leq 3N$ $n \geq k$	$N \leq n \leq 2N$ $0 \leq k \leq N$	$0 \leq k \leq N$	$N \leq n \leq 2N$
Cuboctahedral, generic	$K = 2N$ $n = k$	$n = k = N$	$k = N$	$n = K/2$
Generic cubic A	$K = 3N$	$n > 0, k = 0$	$k = 0$	$n = K/3$
Generic cubic B	$K = 3N - 1$	$n > 0, k = 1$	$k = 1$	$n = (K - 2)/3$
Generic octahedral A	$N = K$	$n = 0, k > 0$	$m = N/2$	$n = 0$
Generic octahedral B	$N = K - 1$	$n = 1, k > 0$	$m = (N-1)/2$	$n = 1$
Elementary cube (B)	$N = 1, K = 3$	$n = 1, k = 0$	$N = 1, k = 0$	$n = 1, K = 3$
Elementary oct. (B)	$N = K = 1$	$n = 0, k = 1$	$N = 1, k = 1$	$n = 0, K = 1$
Atom (A)	$N = K = 0$	$n = k = 0$	$N = k = 0$	$n = K = 0$

Table C.2. Types and notations of all intersecting and generic fcc NPs.

C.4. Properties of Cuboctahedral fcc Nanoparticles

Structural properties characterizing cuboctahedral fcc nanoparticles can be obtained by geometric consideration and simple algebra where we quote only results of the most important quantities. Structure parameters n, k and N, K, according to (C.11), i.e.

$$n = K - N \ , \qquad\qquad k = 3N - K$$
$$2N = n + k \ , \qquad\qquad 2K = 3n + k$$

with constraints listed in Tables C.1, 2 will be used interchangeably and in mixed combinations to simplify formal expressions. Note that according to (C.11c) structure parameters n and k will always be both even or both odd numbers.

As discussed in Section C.3, there are two types of cuboctahedral fcc nanoparticles, those of truncated octahedral and truncated cubic type, which are described by different shapes and, therefore different parameter expressions.

Truncated octahedral fcc NPs are determined by (C.12a)

$$N \leq K \leq 2N \ , \quad 0 \leq n \leq N \ , \quad N \leq k \leq 2N \ , \quad \text{i.e. } n \leq k$$

For geometric convenience we define an alternative structure parameter

$$k' = k - N \tag{C.13}$$

which transforms relations (C.11) to

$$n = K - N \ , \qquad\qquad k' = 2N - K \tag{C.14a}$$

$$N = n + k' \ , \qquad\qquad K = 2n + k' \tag{C.14b}$$

allowing simplifications in some of the subsequent formulas. This will be expressed by an alternative nomenclature of these NPs as fcc(n, k) = **fcc(n, k')$_o$**. Note that according to (C14b) structure parameters K and k' will always be both even or both odd numbers.

Truncated cubic fcc NPs are determined by (C.12b)

$$2N \le K \le 3N \ , \quad N \le n \le 2N \ , \quad 0 \le k \le N \ , \qquad \text{i.e. } k \le n$$

For geometric convenience we define an alternative structure parameter

$$n' = n - N \tag{C.15}$$

which transforms relations (C.11) to

$$n' = K - 2N \ , \qquad\qquad k = 3N - K \tag{C.16a}$$

$$N = n' + k \ , \qquad\qquad K = 3n' + 2k \tag{C.16b}$$

allowing simplifications in some of the subsequent formulas. This will be expressed by an alternative nomenclature of these NPs as fcc(n, k) = **fcc(n', k)$_c$**. Note that according to (C.16a) structure parameters K and n' will always be both even or both odd numbers.

The two types of fcc NPs will be discussed separately in the following.

C.4a. Cuboctahedral fcc Nanoparticles, Truncated Octahedral Type

The number of atoms forming a truncated octahedral fcc(n, k) NP are given by the **volume count** denoted $N_{vol}(n, k)$ where simple algebra yields

$$
\begin{aligned}
N_{vol}(n,k) &= \frac{1}{12}(k+3n+2)\left[(k+3n+2)^2+2\right] - n(n+1)(2n+1) \qquad k \ge n \\
&= \frac{1}{3}(K+1)\left[2(K+1)^2+1\right] - (K-N)(K-N+1)\left[2(K-N)+1\right]
\end{aligned}
\tag{C.17}
$$

with **special cases**

$$
\begin{aligned}
\text{Generic octahedral A} \qquad N_{vol}(0,k) &= \frac{1}{12}(k+2)\left[(k+2)^2+2\right] \\
&= \frac{1}{3}(N+1)\left[2(N+1)^2+1\right]
\end{aligned}
\tag{C.18}
$$

Generic octahedral B
$$N_{vol}(1,k) = \frac{1}{12}(k+5)\left[(k+5)^2+2\right] - 6$$

$$= \frac{1}{3}(N+2)\left[2(N+2)^2+1\right] - 6 \qquad \text{(C.19)}$$

Generic cuboctahedral
$$N_{vol}(n,n) = (2n+1)\left[\frac{5}{3}n(n+1)+1\right]$$

$$= (2N+1)\left[\frac{5}{3}N(N+1)+1\right] \qquad \text{(C.20)}$$

The number of atoms on the outermost facets of a truncated octahedral fcc(n, m) NP (forming the outer polyhedral shell confining the NP) are given by the **facet count** denoted $N_{shell}(\boldsymbol{n}, \boldsymbol{m})$ where simple algebra yields

$$N_{shell}(n,k) = (k+3n)^2 - 6n^2 + 2 = 4K^2 - 6(K-N)^2 + 2 \qquad k \geq n \qquad \text{(C.21)}$$

with **special cases**

Generic octahedral A
$$N_{shell}(0,k) = k^2 + 2 = 4N^2 + 2 \qquad \text{(C.22)}$$

Generic octahedral B
$$N_{shell}(1,k) = (k+3)^2 - 4 = 4(N+1)^2 - 4 \qquad \text{(C.23)}$$

Generic cuboctahedral
$$N_{shell}(n,n) = 10n^2 + 2 = 10N^2 + 2 \qquad \text{(C.24)}$$

The distances between the center of a truncated octahedral fcc(n, k) NP and its outer facet mid-points (**facet distances**) are given by $R_{\{hkl\}}(\boldsymbol{n}, \boldsymbol{k})$, $\{h\,k\,l\} = \{1\,1\,1\}$, $\{1\,0\,0\}$ and which are connected with the polyhedral NP diameters $D_{\{hkl\}}$ according to

$$R_{\{hkl\}}(n,m) = \frac{1}{2}D_{\{hkl\}} \qquad \text{(C.25)}$$

Thus, with (C.2), (C.3), (C.11) and a denoting the lattice constant of the fcc lattice we obtain

$$R_{\{111\}}(n,k) = (K/2)d_{\{111\}} = \frac{a}{4\sqrt{3}}(3n+k) \qquad k \geq n \qquad \text{(C.26)}$$

$$R_{\{100\}}(n,k) = N\,d_{\{100\}} = \frac{a}{4}(n+k) \qquad \text{(C.27)}$$

The distances between the center of a truncated octahedral fcc(n, k) NP and its corners (**corner distances**) are given by $R_c(\boldsymbol{n}, \boldsymbol{k})$ (referring to each of six ($k = n$) or 24 ($k > n$) corners at $\{1\,0\,0\}$ facets) where with (C.11) and a denoting the lattice constant of the fcc lattice

$$R_c(n,k) = \frac{a}{4}\sqrt{(k+n)^2 + 4n^2} = \frac{a}{2}\sqrt{N^2 + (K-N)^2} \qquad k \geq n \qquad \text{(C.28)}$$

The areas of each of the {1 1 1} and {1 0 0} facets of a truncated octahedral fcc(n, k) NP, measured by corresponding corner atoms (**facet areas**), are given by $A_{\{111\}}(n, k)$ (referring to each of eight hexagonal (triangular) {1 1 1} facets) and $A_{\{100\}}(n, k)$ (referring to each of six {1 0 0} facets) where, with (C.2), (C.3), (C.11) and a denoting the lattice constant of the fcc lattice

$$A_{(111)}(n, k) = \frac{\sqrt{3}}{8} a^2 \left[\frac{1}{4}(k + 3n)^2 - 3n^2 \right] = \frac{\sqrt{3}}{8} a^2 \left[K^2 - 3(K - N)^2 \right] \quad \text{(C.29)}$$

$$A_{(100)}(n, k) = \frac{1}{2} a^2 n^2 = \frac{1}{2} a^2 (K - N)^2 \quad \text{(C.30)}$$

C.4b. Cuboctahedral fcc Nanoparticles, Truncated Cubic Type

The number of atoms forming a truncated cubic fcc(n, k) NP are given by the **volume count** denoted $N_{vol}(n, k)$ where simple algebra yields

$$
\begin{aligned}
N_{vol}(n,k) &= \frac{1}{2}(k + n + 2)\left[(k + n)(k + n + 1) + 1\right] - \frac{1}{3}k(k + 2)(2k - 1) \quad n \geq k \\
&= (N + 1)\left[2N(2N + 1) + 1\right] - \frac{1}{3}(3N - K)(3N - K + 2)(2(3N - K) - 1)
\end{aligned}
\quad \text{(C.31)}
$$

with **special cases**

Generic cubic A
$$N_{vol}(n,0) = \frac{1}{2}(n + 2)\left[n(n + 1) + 1\right]$$
$$= (N + 1)\left[2N(2N + 1) + 1\right] \quad \text{(C.32)}$$

Generic cubic B
$$N_{vol}(n,1) = \frac{1}{2}(n + 3)\left[(n + 1)(n + 2) + 1\right] - 1$$
$$= (N + 1)\left[2N(2N + 1) + 1\right] - 1 \quad \text{(C.33)}$$

Generic cuboctahedral
$$N_{vol}(n,n) = (2n + 1)\left[\frac{5}{3}n(n + 1) + 1\right]$$
$$= (2N + 1)\left[\frac{5}{3}N(N + 1) + 1\right] \quad \text{(C.34)}$$

The number of atoms on the outermost facets of a truncated cubic fcc(n, m) NP (forming the outer polyhedral shell confining the NP) are given by the **facet count** denoted $N_{shell}(n, m)$ where simple algebra yields

$$N_{shell}(n,k) = 3(k + n)^2 - 2(k^2 - 1) = 12N^2 - 2\left[(3N - K)^2 - 1\right] \quad n \geq k \quad \text{(C.35)}$$

with **special cases**

Generic cubic A
$$N_{shell}(n,0) = 3n^2 + 2 = 3(K - N)^2 + 2 \quad \text{(C.36)}$$

Generic cubic B $\qquad N_{shell}(n,1) = 3(n+1)^2 = 12N^2$ (C.37)

Generic cuboctahedral $\qquad N_{shell}(n,n) = 10n^2 + 2 = 10N^2 + 2$ (C.38)

The distances between the center of a truncated cubic fcc(n, k) NP and its outer facet midpoints (**facet distances**) are given by $R_{\{hkl\}}(\boldsymbol{n, k})$, $\{h\,k\,l\} = \{1\,1\,1\}$, $\{1\,0\,0\}$ and which are connected with the polyhedral NP diameters $D_{\{hkl\}}$ according to

$$R_{\{hkl\}}(n,m) = \frac{1}{2}D_{\{hkl\}}$$ (C.39)

Thus, with (C.2), (C.3), (C.11) and a denoting the lattice constant of the fcc lattice we obtain

$$R_{\{111\}}(n,k) = (K/2)d_{\{111\}} = \frac{a}{4\sqrt{3}}(3n+k) \qquad n \geq k$$ (C.40)

$$R_{\{100\}}(n,k) = N d_{\{100\}} = \frac{a}{4}(n+k)$$ (C.41)

The distances between the center of a truncated cubic fcc(n, k) NP and its corners (**corner distances**) are given by $R_c(\boldsymbol{n, k})$ (referring to each of six ($n = k$) or 24 ($n > k$) corners at $\{1\,0\,0\}$ facets) where with (C.11) and a denoting the lattice constant of the fcc lattice

$$R_c(n,k) = \frac{a}{4}\sqrt{3(k+n)^2 - 4kn} = \frac{a}{2}\sqrt{(2N-K)^2 + 2N^2} \qquad n \geq k$$ (C.42)

The areas of each of the $\{1\,1\,1\}$ and $\{1\,0\,0\}$ facets of a truncated cubic fcc(n, k) NP, measured by corresponding corner atoms (**facet areas**), are given by $A_{\{111\}}(\boldsymbol{n, k})$ (referring to each of eight hexagonal (triangular) $\{1\,1\,1\}$ facets) and $A_{\{100\}}(\boldsymbol{n, k})$ (referring to each of six $\{1\,0\,0\}$ facets) where, with (C.2), (C.3), (C.11) and a denoting the lattice constant of the fcc lattice

$$A_{(111)}(n,\ k) = \frac{\sqrt{3}}{8}a^2k^2 = \frac{\sqrt{3}}{8}a^2(3N-K)^2$$ (C.43)

$$A_{(100)}(n,\ k) = \frac{a^2}{4}\left[(n+k)^2 - 2k^2\right] = a^2\left[N^2 - \frac{1}{2}(3N-K)^2\right]$$ (C.44)

III. Conclusion

The present work gives a full account of the shape and structure of ideal nanoparticles (NPs) forming compact polyhedral sections of the ideal cubic lattice where simple, body centered, and face centered variants are considered. We have studied particles of O_h symmetry which are confined by facets of densest and second densest monolayers of the lattice reflecting Miller index families {1 0 0}, {1 1 0} for sc and bcc as well as {1 1 1}, {1 0 0} for fcc. The structure evaluation identifies different types of generic NPs which serve for the definition of general polyhedral NPs. These can be classified according to integer valued structure parameters N, M (, K) which are connected with particle diameters along corresponding facet normal directions reflecting {$h\,k\,l$} monolayer families of the underlying lattice. An alternative classification is based on parameters n, m (, k) which can describe characteristic lengths of facet edges of the NPs where the parameters of the two classification are connected by linear transformations. Detailed structural properties of the general polyhedral NPs, such as shape, size, and surfaces, are discussed in analytical and numerical detail with visualization of characteristic examples.

Clearly, the present results deal only with ideal cubic NPs and cannot account for all possible structures of the most general metal nanoparticles observed, for example, by electron microscopy [a13]. Realistic NPs may exhibit very different shapes, including less compact particles, and symmetry, including local structural disorder and deviations from (incompatibility with) crystal lattice structure in their inner core. This can only be examined in case-by-case studies where exact quantitative results are difficult to obtain. However, the present results can be used in an approximate way to estimate typical particle sizes of metal NPs as well as for a repository of possible structures of compact NPs with internal cubic lattice.

IV. References

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V. Supplementary Information

S.1. Symmetry Centers

The cubic NPs, sc(n, m), bcc(n, m), and fcc(n, m) of O_h symmetry contain atoms or high symmetry voids at their center depending on the lattice type and on the N, M, K, n, m, k as described in the following.

The **simple cubic** lattice offers two different centers of O_h symmetry, an atom site and a high symmetry void as shown in Fig. S.1.

(a)   (b)
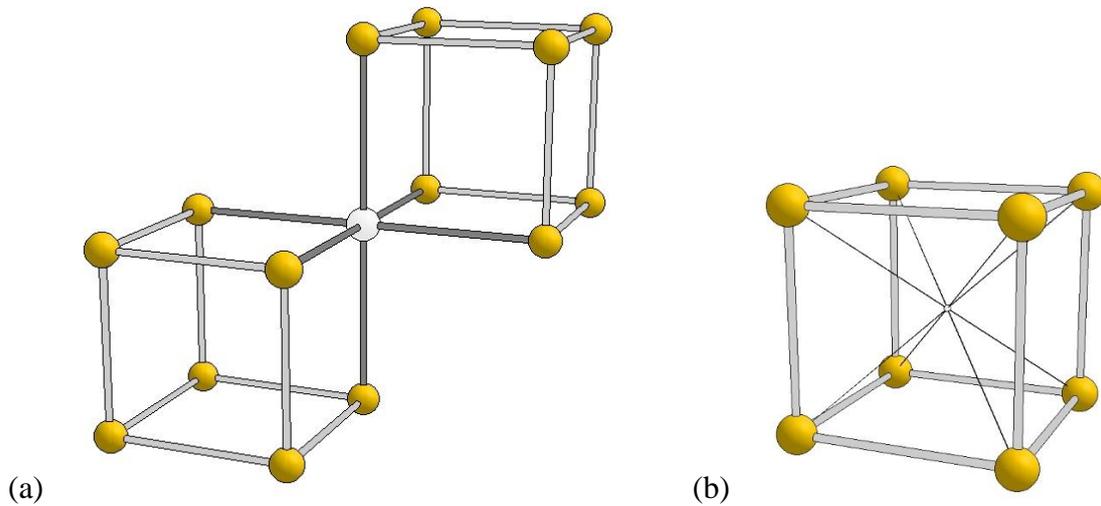
Figure S.1. O_h symmetry centers of the simple cubic lattice, (a) center at atom site, (b) center at high symmetry void. The centers are emphasized by white balls and connected with their nearest neighbor atoms by dark sticks and black lines, respectively.

This discriminates between two types of sc[N, M], sc(n, m) NPs, those about an atom center and those about a high symmetry void, as discussed in Sec. II.A.1 and spelled out in the following table.

Center type	N	M	n	m
Atom	even	any	even	any
Void	odd	any	odd	any

$n = 2M - N$, $m = N - M$

The **body centered cubic** lattice offers only one center of O_h symmetry which coincides with an atom site as shown in Fig. S.2.
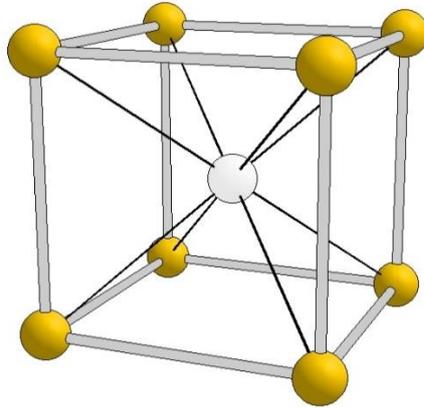
Figure S.2. O_h symmetry center of the body centered cubic lattice at atom site. The center is emphasized by a white ball and connected with its nearest neighbor atoms by black lines.

This allows for only one type of bcc[N, M], bcc(n, m) NPs, about an atom center as discussed in Sec. II.B.1 where $n = 2M - N$, $m = N - M$.

The **face centered cubic** lattice offers two different centers of O_h symmetry, an atom site and a high symmetry void as shown in Fig. S.3.

(a)   (b)
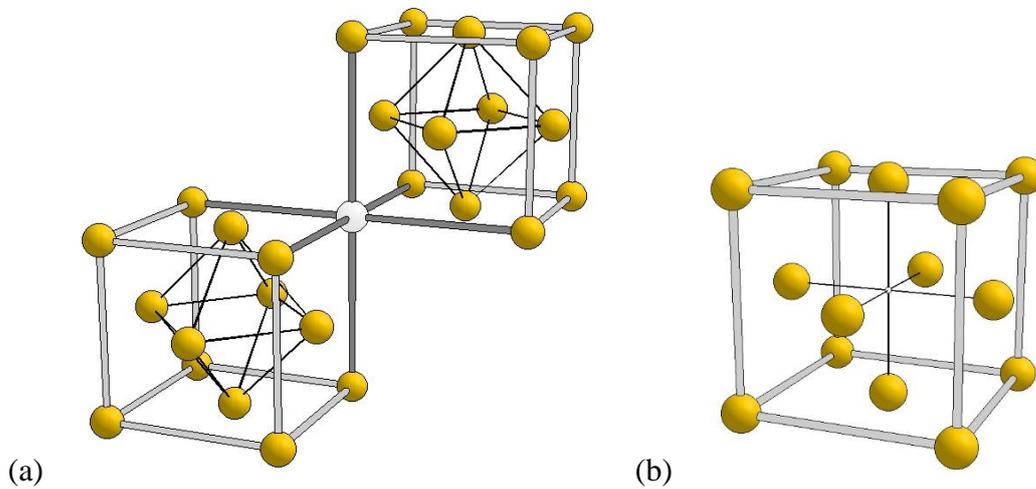
Figure S.3. O_h symmetry centers of the face centered cubic lattice, (a) center at atom site, (b) center at high symmetry void. The centers are emphasized by white balls and connected with their nearest neighbor atoms by dark sticks and black lines, respectively.

This discriminates between two types of octahedral and cubic fcc[N, K], fcc(n, k) NPs, about an atom center and about a high symmetry void, as discussed in Sec. II.C.1 and spelled out in the following table.

Center type	N	K	n	k
Atom	even	even	even	even
Atom	odd	even	odd	odd
Void	even	odd	odd	odd
Void	odd	odd	even	even

$n = K - N$, $k = 3N - K$

S.2. Nanoparticle Peeling and Dressing

Taking off all atoms of the outermost {hkl} facet layer of a general cubic NP, denoted by structure parameters [N, M], (n, m) or [N, K], (n, k), ({hkl} **peeling**) leads to a smaller NP, denoted by [N', M'], (n', m') or [N', K'], (n', k') whose structure can be evaluated analytically. Further, adding all atoms from possible nearest outermost {hkl} monolayer facets ({hkl} **dressing**) leads to a larger NP and can also be evaluated analytically as discussed below. Successive peeling steps can reduce the cubic NP to a primitive (0, 0), (1, 0), or (0, 1) NP. This provides a detailed analysis of the internal structure of the NP.

S.2.1. Cubo-rhombic sc Nanoparticles

Peeling and dressing a cubo-rhombic sc[N, M], sc(n, m) NP of simple cubic lattice structure can be expressed by transformed structure parameters N', M', n', m' which depend on the initial parameters M, N and are listed in the following tables. For the sake of brevity the prefix "sc" has been omitted in all NP notations.

- **{1 0 0} peeling /dressing**

Nanoparticle	Peeled sc NP $[N', M'] / (n', m')$	Dressed sc NP $[N', M'] / (n', m')$
Cubo-rhombic $M + 2 \leq N \leq 2M - 2$	$[N - 2, M] / (n + 2, m - 2)$	$[N + 2, M] / (n - 2, m + 2)$
Generic cubic $N = M, \ m = 0$	$[N - 2, M - 2] / (n - 2, 0)$	$[N + 2, M] / (n - 2, 2)$
Cubo-rhombic $N = M + 1, \ m = 1$	$[N - 2, M - 1] / (n, 0)$	$[N + 2, M] / (n - 2, 3)$
Generic rhombic A $N = 2M, \ n = 0$	$[N - 2, M] / (2, m - 2)$	$[N, M] / (0, m)$
Generic rhombic B $N = 2M - 1, \ n = 1$	$[N - 2, M] / (3, m - 2)$	$[N + 2, M + 1] / (1, m + 1)$

$n = 2M - N \ , \quad m = N - M \ , \quad N = n + 2m \ , \quad M = n + m \ , \quad M \leq N \leq 2M$

- **{1 1 0} peeling /dressing**

Nanoparticle	Peeled sc NP $[N', M'] / (n', m')$	Dressed sc NP $[N', M'] / (n', m')$
Cubo-rhombic $M \leq N \leq 2M - 2$	$[N, M - 1] / (n - 2, m + 1)$	$[N, M + 1] / (n + 2, m - 1)$
Generic cubic $N = M, \ m = 0$	$[N, M - 1] / (n - 2, 1)$	$[N, M] / (n, 0)$
Generic rhombic A $N = 2M, \ n = 0$	$[N - 2, M - 1] / (0, m - 1)$	$[N, M + 1] / (2, m - 1)$
Generic rhombic B $N = 2M - 1, \ n = 1$	$[N - 2, M - 1] / (1, m - 1)$	$[N, M + 1] / (3, m - 1)$

$n = 2M - N \ , \quad m = N - M \ , \quad N = n + 2m \ , \quad M = n + m \ , \quad M \leq N \leq 2M$

- **shell (joint {1 0 0} and {1 1 0}) peeling /dressing**

Nanoparticle	Peeled sc NP $[N', M'] / (n', m')$	Dressed sc NP $[N', M'] / (n', m')$
Cubo-rhombic $M + 2 \leq N \leq 2M - 1$	$[N - 2, M - 1] / (n, m - 1)$	$[N + 2, M + 1] / (n, m + 1)$
Generic cubic $N = M, \ m = 0$	$[N - 2, M - 2] / (n - 2, 0)$	$[N + 2, M + 1] / (n, 1)$
Generic rhombic A $N = 2M, \ n = 0$	$[N - 2, M - 1] / (0, m - 1)$	$[N + 2, M + 1] / (0, m + 1)$
Generic rhombic B $N = 2M - 1, \ n = 1$	$[N - 2, M - 1] / (1, m - 1)$	$[N + 2, M + 1] / (1, m + 1)$

$n = 2M - N \ , \quad m = N - M \ , \quad N = n + 2m \ , \quad M = n + m \ , \quad M \leq N \leq 2M$

S.2.2. Cubo-rhombic bcc Nanoparticles

Peeling and dressing a cubo-rhombic bcc[N, M], bcc(n, m) NP of body centered cubic lattice structure can be expressed by transformed structure parameters N', M', n', m' which depend on the initial parameters M, N and are listed in the following tables. For the sake of brevity the prefix "bcc" has been omitted in all NP notations.

- **{1 0 0} peeling /dressing**

Nanoparticle	Peeled bcc NP [N', M'] / (n', m')	Dressed bcc NP [N', M'] / (n', m')
Cubo-rhombic $M + 1 \leq N \leq 2M - 1$	[$N - 1$, M] / ($n + 1$, $m - 1$)	[$N + 1$, M] / ($n - 1$, $m + 1$)
Generic cubic $N = M$, $m = 0$	[$N - 1$, $M - 1$] / ($n - 1$, 0)	[$N + 1$, M] / ($n - 1$, 1)
Generic rhombic $N = 2M$, $n = 0$	[$N - 1$, M] / (1, $m - 1$)	[N, M] / (0, m)

$n = 2M - N$, $m = N - M$, $N = n + 2m$, $M = n + m$, $M \leq N \leq 2M$

- **{1 1 0} peeling /dressing**

Nanoparticle	Peeled bcc NP [N', M'] / (n', m')	Dressed bcc NP [N', M'] / (n', m')
Cubo-rhombic $M + 1 \leq N \leq 2M - 2$	[N, $M - 1$] / ($n - 2$, $m + 1$)	[N, $M + 1$] / ($n + 2$, $m - 1$)
Generic cubic $N = M$, $m = 0$	[N, $M - 1$] / ($n - 2$, 1)	[N, M] / (n, 0)
Generic rhombic $N = 2M$, $n = 0$	[$N - 2$, $M - 1$] / (0, $m - 1$)	[N, $M + 1$] / (2, $m - 1$)

$n = 2M - N$, $m = N - M$, $N = n + 2m$, $M = n + m$, $M \leq N \leq 2M$

- **shell (joint {1 0 0} and {1 1 0}) peeling /dressing**

Nanoparticle	Peeled bcc NP [N', M'] / (n', m')	Dressed bcc NP [N', M'] / (n', m')
Cubo-rhombic $M + 1 \leq N \leq 2M - 1$	[$N - 1$, $M - 1$] / ($n - 1$, m)	[$N + 1$, $M + 1$] / ($n + 1$, m)
Generic cubic $N = M$, $m = 0$	[$N - 1$, $M - 1$] / ($n - 1$, 0)	[$N + 1$, $M + 1$] / ($n + 1$, 0)
Generic rhombic $N = 2M$, $n = 0$	[$N - 2$, $M - 1$] / (0, $m - 1$)	[$N + 1$, $M + 1$] / (1, m)

$n = 2M - N$, $m = N - M$, $N = n + 2m$, $M = n + m$, $M \leq N \leq 2M$

S.2.3. Cuboctahedral fcc Nanoparticles

Peeling and dressing a cuboctahedral fcc[N, K], fcc(n, k) NP of face centerd cubic lattice structure can be expressed by transformed structure parameters N', K', n', k' which depend on the initial parameters M, K and are listed in the following tables. For the sake of brevity the prefix "fcc" has been omitted in all NP notations.

As discussed in Sec. C.3, there are two types of face centered cubic NPs which are distinguished by their shape, truncated octahedral and truncated cubic fcc[N, K], fcc(n, k), with N, K, n, k determined by relations (C.12a) and (C.12b), respectively. Peeling and dressing induce transitions between the two types, cubic to octahedral for peeling and octahedral to cubic for dressing, but do not affect corresponding transformations N, K, n, k to N', K', n', k'.

- **{1 0 0} peeling /dressing**

Nanoparticle	Peeled fcc NP [N', K'] / (n', k')	Dressed fcc NP [N', K'] / (n', k')
Cuboctahedral $N \le K \le 3N - 3$	[N -1, K] / ($n + 1$, k - 3)	[$N + 1$, K] / ($n - 1$, $k + 3$)
Generic cubic A $K = 3N$, $k = 0$	[$N - 1$, K- 4] / ($n - 3$, 1)	[$N + 1$, K] / ($n - 1$, 3)
Generic cubic B $K = 3N - 1$, $k = 1$	[$N - 1$, $K - 2$] / ($n - 1$, 0)	[$N + 1$, K] / ($n - 1$, 4)
Generic cubic C $K = 3N - 2$, $k = 2$	[$N - 1$, $K - 2$] / ($n - 1$, 1)	[$N + 1$, K] / ($n - 1$, 5)
Generic octahedral A $K = N$, $n = 0$	[$N - 1$, K] / (1, k - 3)	[N, K] / (0, k)
Generic octahedral B $K = N + 1$, $n = 1$	[$N - 1$, K] / (2, k - 3)	[$N + 1$, K] / (0, $k + 3$)
Generic cuboctahedral $K = 2N$, $n = k$	[$N - 1$, K] / ($n + 1$, k - 3)	[$N + 1$, K] / ($n - 1$, $k + 3$)

$n = K - N$, $k = 3N - K$, $2N = n + k$, $2K = 3n + k$, $N \le K \le 3N$

- **{1 1 1} peeling /dressing**

Nanoparticle	Peeled fcc NP $[N', K'] / (n', k')$	Dressed fcc NP $[N', K'] / (n', k')$
Cuboctahedral $N + 2 \leq K \leq 3N - 2$	$[N, K - 2] / (n - 2, k + 2)$	$[N, K + 2] / (n + 2, k - 2)$
Generic cubic A $K = 3N, \ k = 0$	$[N, K - 2] / (n - 2, 2)$	$[N, K] / (n, 0)$
Generic cubic B $K = 3N - 1, \ k = 1$	$[N, K - 2] / (n - 2, 3)$	$[N, K] / (n, 1)$
Generic cubic C $K = 3N - 2, \ k = 2$	$[N, K - 2] / (n - 2, 4)$	$[N, K + 2] / (n + 2, 0)$
Generic octahedral A $K = N, \ n = 0$	$[N - 2, K - 2] / (0, k - 4)$	$[N, K + 2] / (2, k - 2)$
Generic octahedral B $K = N + 1, \ n = 1$	$[N - 1, K - 2] / (0, k - 1)$	$[N, K + 2] / (3, k - 2)$
Generic cuboctahedral $K = 2N, \ n = k$	$[N, K - 2] / (n - 2, k + 2)$	$[N, K + 2] / (n + 2, k - 2)$

$n = K - N \ , \qquad k = 3N - K \ , \qquad 2N = n + k \ , \qquad 2K = 3n + k \ , \quad N \leq K \leq 3N$

- **shell (joint {1 0 0} and {1 1 1}) peeling /dressing**

Nanoparticle	Peeled fcc NP $[N', K'] / (n', k')$	Dressed fcc NP $[N', K'] / (n', k')$
Cuboctahedral $N + 1 \leq K \leq 3N - 1$	$[N - 1, K - 2] / (n - 1, k - 1)$	$[N + 1, K + 2] / (n + 1, k + 1)$
Generic cubic A $K = 3N, \ k = 0$	$[N - 1, K - 4] / (n - 3, 1)$	$[N + 1, K + 2] / (n + 1, 1)$
Generic cubic B $K = 3N - 1, \ k = 1$	$[N - 1, K - 2] / (n - 1, 0)$	$[N + 1, K + 2] / (n + 1, 2)$
Generic cubic C $K = 3N - 2, \ k = 2$	$[N - 1, K - 2] / (n - 1, 1)$	$[N + 1, K + 2] / (n + 1, 3)$
Generic octahedral A $K = N, \ n = 0$	$[N - 2, K - 2] / (0, k - 4)$	$[N + 1, K + 2] / (1, k + 1)$
Generic octahedral B $K = N + 1, \ n = 1$	$[N - 1, K - 2] / (0, k - 1)$	$[N + 1, K + 2] / (2, k + 1)$
Generic cuboctahedral $K = 2N, \ n = k$	$[N - 1, K - 2] / (n - 1, k - 1)$	$[N + 1, K + 2] / (n + 1, k + 1)$

$n = K - N \ , \qquad k = 3N - K \ , \qquad 2N = n + k \ , \qquad 2K = 3n + k \ , \quad N \leq K \leq 3N$

S.3. Numerical Tables

S.3.1. Cubo-rhombic sc Nanoparticles

Table 1.1. Notation of a non-generic cubo-rhombic NP sc[N, M], sc(n, m) for given n, m according to $N = n + 2m$, $M = n + m$. Structure parameters N, M describe the two generic envelope NPs, cubic sc[N, 0] and rhombic A sc(0, M] (n even) or rhombic B sc(1, M) (n odd) by polyhedral diameters, see Sec. A.3. In contrast, n, m characterize the deviation of the cubo-rhombic NP sc[N, M] from its generic envelope NPs.

List of [N, M]

$m\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	[0, 0]	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]	[8, 8]	[9, 9]	[10,10]	[11,11]
1	[2, 1]	[3, 2]	[4, 3]	[5, 4]	[6, 5]	[7, 6]	[8, 7]	[9, 8]	[10, 9]	[11,10]	[12,11]	[13,12]
2	[4, 2]	[5, 3]	[6, 4]	[7, 5]	[8, 6]	[9, 7]	[10, 8]	[11, 9]	[12,10]	[13,11]	[14,12]	[15,13]
3	[6, 3]	[7, 4]	[8, 5]	[9, 6]	[10, 7]	[11, 8]	[12, 9]	[13,10]	[14,11]	[15,12]	[16,13]	[17,14]
4	[8, 4]	[9, 5]	[10, 6]	[11, 7]	[12, 8]	[13, 9]	[14,10]	[15,11]	[16,12]	[17,13]	[18,14]	[19,15]
5	[10, 5]	[11, 6]	[12, 7]	[13, 8]	[14, 9]	[15,10]	[16,11]	[17,12]	[18,13]	[19,14]	[20,15]	[21,16]
6	[12, 6]	[13, 7]	[14, 8]	[15, 9]	[16,10]	[17,11]	[18,12]	[19,13]	[20,14]	[21,15]	[22,16]	[23,17]
7	[14, 7]	[15, 8]	[16, 9]	[17,10]	[18,11]	[19,12]	[20,13]	[21,14]	[22,15]	[23,16]	[24,17]	[25,18]
8	[16, 8]	[17, 9]	[18,10]	[19,11]	[20,12]	[21,13]	[22,14]	[23,15]	[24,16]	[25,17]	[26,18]	[27,19]
9	[18, 9]	[19,10]	[20,11]	[21,12]	[22,13]	[23,14]	[24,15]	[25,16]	[26,17]	[27,18]	[28,19]	[29,20]
10	[20,10]	[21,11]	[22,12]	[23,13]	[24,14]	[25,15]	[26,16]	[27,17]	[28,18]	[29,19]	[30,20]	[31,21]
11	[22,11]	[23,12]	[24,13]	[25,14]	[26,15]	[27,16]	[28,17]	[29,18]	[30,19]	[31,20]	[32,21]	[33,22]

Table 1.2. Number of atoms inside the volume of an sc(n, m) NP, $N_{vol}(n, m)$, (volume count) as defined by (A.17 - 20).

List of $N_{vol}(n, m)$

$m\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	1	8	27	64	125	216	343	512	729	1000	1331	1728
1	7	32	81	160	275	432	637	896	1215	1600	2057	2592
2	33	88	179	312	493	728	1023	1384	1817	2328	2923	3608
3	87	184	329	528	787	1112	1509	1984	2543	3192	3937	4784
4	185	336	547	824	1173	1600	2111	2712	3409	4208	5115	6136
5	335	552	841	1208	1659	2200	2837	3576	4423	5384	6465	7672
6	553	848	1227	1696	2261	2928	3703	4592	5601	6736	8003	9408
7	847	1232	1713	2296	2987	3792	4717	5768	6951	8272	9737	11352
8	1233	1720	2315	3024	3853	4808	5895	7120	8489	10008	11683	13520
9	1719	2320	3041	3888	4867	5984	7245	8656	10223	11952	13849	15920
10	2321	3048	3907	4904	6045	7336	8783	10392	12169	14120	16251	18568
11	3047	3912	4921	6080	7395	8872	10517	12336	14335	16520	18897	21472

Table 1.3. Number of atoms on the outermost facets of an sc(n, m) NP, $N_{\text{shell}}(n, m)$, (facet count) as defined by (A.21 - 24).

List of $N_{\text{shell}}(n, m)$

$m\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	--	8	26	56	98	152	218	296	386	488	602	728
1	6	24	54	96	150	216	294	384	486	600	726	864
2	26	56	98	152	218	296	386	488	602	728	866	1016
3	54	96	150	216	294	384	486	600	726	864	1014	1176
4	98	152	218	296	386	488	602	728	866	1016	1178	1352
5	150	216	294	384	486	600	726	864	1014	1176	1350	1536
6	218	296	386	488	602	728	866	1016	1178	1352	1538	1736
7	294	384	486	600	726	864	1014	1176	1350	1536	1734	1944
8	386	488	602	728	866	1016	1178	1352	1538	1736	1946	2168
9	486	600	726	864	1014	1176	1350	1536	1734	1944	2166	2400
10	602	728	866	1016	1178	1352	1538	1736	1946	2168	2402	2648
11	726	864	1014	1176	1350	1536	1734	1944	2166	2400	2646	2904

Table 1.4. Corner distances, $R_{c1}(n, m)$, defining the distances from the center of a simple cubic sc(n, m) NP to its 24 ($n > 0$) and 6 ($n = 0$) corners, respectively, at {1 0 0} facets and $R_{c2}(n, m)$, defining the distances to its 8 (m even) and 24 (m odd) corners, respectively, at {1 1 0} (and 8 possible {1 1 1}) facets. The distances are defined by (A.29), (A.30) and all radii are normalized by the lattice constant a of the sc lattice.

List of $R_{c1}(n, m) / a$

$m\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526
1	1.000	1.658	2.449	3.279	4.123	4.975	5.831	6.690	7.550	8.411	9.274	10.137
2	2.000	2.598	3.317	4.093	4.899	5.723	6.557	7.399	8.246	9.097	9.950	10.805
3	3.000	3.571	4.243	4.975	5.745	6.538	7.348	8.170	9.000	9.836	10.677	11.522
4	4.000	4.555	5.196	5.895	6.633	7.399	8.185	8.986	9.798	10.618	11.446	12.278
5	5.000	5.545	6.164	6.837	7.550	8.292	9.055	9.836	10.630	11.435	12.247	13.067
6	6.000	6.538	7.141	7.794	8.485	9.206	9.950	10.712	11.489	12.278	13.077	13.883
7	7.000	7.533	8.124	8.761	9.434	10.137	10.863	11.608	12.369	13.143	13.928	14.722
8	8.000	8.529	9.110	9.734	10.392	11.079	11.790	12.520	13.266	14.027	14.799	15.580
9	9.000	9.526	10.100	10.712	11.358	12.031	12.728	13.444	14.177	14.925	15.684	16.454
10	10.000	10.524	11.091	11.694	12.329	12.990	13.675	14.379	15.100	15.835	16.583	17.342
11	11.000	11.522	12.083	12.679	13.304	13.955	14.629	15.322	16.031	16.756	17.493	18.241

List of $R_{c2}(n, m) / a$

m\n	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526
1	1.000	1.658	2.449	3.279	4.123	4.975	5.831	6.690	7.550	8.411	9.274	10.137
2	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258
3	2.449	3.279	4.123	4.975	5.831	6.690	7.550	8.411	9.274	10.137	11.000	11.864
4	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990
5	4.123	4.975	5.831	6.690	7.550	8.411	9.274	10.137	11.000	11.864	12.728	13.592
6	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722
7	5.831	6.690	7.550	8.411	9.274	10.137	11.000	11.864	12.728	13.592	14.457	15.322
8	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454
9	7.550	8.411	9.274	10.137	11.000	11.864	12.728	13.592	14.457	15.322	16.186	17.051
10	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454	17.321	18.187
11	9.274	10.137	11.000	11.864	12.728	13.592	14.457	15.322	16.186	17.051	17.916	18.782

S.3.2. Cubo-rhombic bcc Nanoparticles

Table 2.1. Notation of a non-generic cubo-rhombic NP bcc[N, M], bcc(n, m) for given n, m according to $N = n + 2m$, $M = n + m$. Structure parameters N, M describe the two generic envelope NPs, cubic sc[N, 0) and rhombic sc(0, M] by polyhedral diameters, see Sec. B.3. In contrast, n, m characterize the deviation of the cubo-rhombic NP bcc[N, M] from its generic envelope NPs.

List of $N : M$

m\n	0	1	2	3	4	5	6	7	8	9	10	11
0	[0, 0]	[1, 1]	[2, 2]	[3, 3]	[4, 4]	[5, 5]	[6, 6]	[7, 7]	[8, 8]	[9, 9]	[10,10]	[11,11]
1	[2, 1]	[3, 2]	[4, 3]	[5, 4]	[6, 5]	[7, 6]	[8, 7]	[9, 8]	[10, 9]	[11,10]	[12,11]	[13,12]
2	[4, 2]	[5, 3]	[6, 4]	[7, 5]	[8, 6]	[9, 7]	[10, 8]	[11, 9]	[12,10]	[13,11]	[14,12]	[15,13]
3	[6, 3]	[7, 4]	[8, 5]	[9, 6]	[10, 7]	[11, 8]	[12, 9]	[13,10]	[14,11]	[15,12]	[16,13]	[17,14]
4	[8, 4]	[9, 5]	[10, 6]	[11, 7]	[12, 8]	[13, 9]	[14,10]	[15,11]	[16,12]	[17,13]	[18,14]	[19,15]
5	[10, 5]	[11, 6]	[12, 7]	[13, 8]	[14, 9]	[15,10]	[16,11]	[17,12]	[18,13]	[19,14]	[20,15]	[21,16]
6	[12, 6]	[13, 7]	[14, 8]	[15, 9]	[16,10]	[17,11]	[18,12]	[19,13]	[20,14]	[21,15]	[22,16]	[23,17]
7	[14, 7]	[15, 8]	[16, 9]	[17,10]	[18,11]	[19,12]	[20,13]	[21,14]	[22,15]	[23,16]	[24,17]	[25,18]
8	[16, 8]	[17, 9]	[18,10]	[19,11]	[20,12]	[21,13]	[22,14]	[23,15]	[24,16]	[25,17]	[26,18]	[27,19]
9	[18, 9]	[19,10]	[20,11]	[21,12]	[22,13]	[23,14]	[24,15]	[25,16]	[26,17]	[27,18]	[28,19]	[29,20]
10	[20,10]	[21,11]	[22,12]	[23,13]	[24,14]	[25,15]	[26,16]	[27,17]	[28,18]	[29,19]	[30,20]	[31,21]
11	[22,11]	[23,12]	[24,13]	[25,14]	[26,15]	[27,16]	[28,17]	[29,18]	[30,19]	[31,20]	[32,21]	[33,22]

Table 2.2. Number of atoms inside the volume of a bcc(n, m) NP, $N_{\text{vol}}(n, m)$, (volume count) as defined by (B.12 - 14).

List of $N_{\text{vol}}(n, m)$

m\n	0	1	2	3	4	5	6	7	8	9	10	11
0	1	9	35	91	189	341	559	855	1241	1729	2331	3059
1	15	59	145	285	491	775	1149	1625	2215	2931	3785	4789
2	65	169	339	587	925	1365	1919	2599	3417	4385	5515	6819
3	175	363	641	1021	1515	2135	2893	3801	4871	6115	7545	9173
4	369	665	1075	1611	2285	3109	4095	5255	6601	8145	9899	11875
5	671	1099	1665	2381	3259	4311	5549	6985	8631	10499	12601	14949
6	1105	1689	2435	3355	4461	5765	7279	9015	10985	13201	15675	18419
7	1695	2459	3409	4557	5915	7495	9309	11369	13687	16275	19145	22309
8	2465	3433	4611	6011	7645	9525	11663	14071	16761	19745	23035	26643
9	3439	4635	6065	7741	9675	11879	14365	17145	20231	23635	27369	31445
10	4641	6089	7795	9771	12029	14581	17439	20615	24121	27969	32171	36739
11	6095	7819	9825	12125	14731	17655	20909	24505	28455	32771	37465	42549

Table 2.3. Number of atoms on the outermost facets of a bcc(n, m) NP, $N_{\text{shell}}(n, m)$, (facet count) as defined by (B.15 - 17).

List of $N_{\text{shell}}(n, m)$

m\n	0	1	2	3	4	5	6	7	8	9	10	11
0	--	8	26	56	98	152	218	296	386	488	602	728
1	14	44	86	140	206	284	374	476	590	716	854	1004
2	50	104	170	248	338	440	554	680	818	968	1130	1304
3	110	188	278	380	494	620	758	908	1070	1244	1430	1628
4	194	296	410	536	674	824	986	1160	1346	1544	1754	1976
5	302	428	566	716	878	1052	1238	1436	1646	1868	2102	2348
6	434	584	746	920	1106	1304	1514	1736	1970	2216	2474	2744
7	590	764	950	1148	1358	1580	1814	2060	2318	2588	2870	3164
8	770	968	1178	1400	1634	1880	2138	2408	2690	2984	3290	3608
9	974	1196	1430	1676	1934	2204	2486	2780	3086	3404	3734	4076
10	1202	1448	1706	1976	2258	2552	2858	3176	3506	3848	4202	4568
11	1454	1724	2006	2300	2606	2924	3254	3596	3950	4316	4694	5084

Table 2.4. Corner distances, $R_{c1}(n, m)$, defining the distances from the center of a body centered cubic bcc(n, m) NP to its 24 ($n > 0$) and 6 ($n = 0$) corners, respectively, at {1 0 0} facets and $R_{c2}(n, m)$, defining the distances to its 8 corners at {1 1 0} facets. The distances are defined by (B.22), (B.23) and all radii are normalized by the lattice constant a of the sc lattice.

List of $R_{c1}(n, m) / a$

$m \backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526
1	1.000	1.658	2.449	3.279	4.123	4.975	5.831	6.690	7.550	8.411	9.274	10.137
2	2.000	2.598	3.317	4.093	4.899	5.723	6.557	7.399	8.246	9.097	9.950	10.805
3	3.000	3.571	4.243	4.975	5.745	6.538	7.348	8.170	9.000	9.836	10.677	11.522
4	4.000	4.555	5.196	5.895	6.633	7.399	8.185	8.986	9.798	10.618	11.446	12.278
5	5.000	5.545	6.164	6.837	7.550	8.292	9.055	9.836	10.630	11.435	12.247	13.067
6	6.000	6.538	7.141	7.794	8.485	9.206	9.950	10.712	11.489	12.278	13.077	13.883
7	7.000	7.533	8.124	8.761	9.434	10.137	10.863	11.608	12.369	13.143	13.928	14.722
8	8.000	8.529	9.110	9.734	10.392	11.079	11.790	12.520	13.266	14.027	14.799	15.580
9	9.000	9.526	10.100	10.712	11.358	12.031	12.728	13.444	14.177	14.925	15.684	16.454
10	10.000	10.524	11.091	11.694	12.329	12.990	13.675	14.379	15.100	15.835	16.583	17.342
11	11.000	11.522	12.083	12.679	13.304	13.955	14.629	15.322	16.031	16.756	17.493	18.241

List of $R_{c2}(n, m) / a$

$m \backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526
1	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392
2	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258
3	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124
4	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990
5	4.330	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856
6	5.196	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722
7	6.062	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588
8	6.928	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454
9	7.794	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454	17.321
10	8.660	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454	17.321	18.187
11	9.526	10.392	11.258	12.124	12.990	13.856	14.722	15.588	16.454	17.321	18.187	19.053

S.3.3a. Cuboctahedral fcc Nanoparticles, Truncated Octahedral Type

Table 3.1. Notation of a non-generic cuboctahedral NP fcc[N, K], fcc(n, k) for given n, k according to $2N = n + k$, $2K = 3n + k$. Structure parameters N, K describe the two generic envelope NPs, cubic fcc[N, 0], fcc[N, 1] and octahedral sc(0, K], sc(1, K] by polyhedral diameters, see Sec. C.3. In contrast, n, k characterize the deviation of the cuboctahedral NP fcc[N, M] from its generic envelope NPs.

For fcc[N, K] NPs of the octahedral type, i.e. if $N \le K \le 2N$, $k \ge n$, it is meaningful to use an auxiliary index k' with $k' = (k - n)/2$ resulting in a notation fcc(n, k')$_o$, see Sec. C.3, and yielding

$$[N, K]: \quad N = n + k', \quad K = 2n + k'$$

List of [N, K]

$k'\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	[0, 0]	[1, 2]	[2, 4]	[3, 6]	[4, 8]	[5,10]	[6,12]	[7,14]	[8,16]	[9,18]	[10,20]	[11,22]
1	[1, 1]	[2, 3]	[3, 5]	[4, 7]	[5, 9]	[6,11]	[7,13]	[8,15]	[9,17]	[10,19]	[11,21]	[12,23]
2	[2, 2]	[3, 4]	[4, 6]	[5, 8]	[6,10]	[7,12]	[8,14]	[9,16]	[10,18]	[11,20]	[12,22]	[13,24]
3	[3, 3]	[4, 5]	[5, 7]	[6, 9]	[7,11]	[8,13]	[9,15]	[10,17]	[11,19]	[12,21]	[13,23]	[14,25]
4	[4, 4]	[5, 6]	[6, 8]	[7,10]	[8,12]	[9,14]	[10,16]	[11,18]	[12,20]	[13,22]	[14,24]	[15,26]
5	[5, 5]	[6, 7]	[7, 9]	[8,11]	[9,13]	[10,15]	[11,17]	[12,19]	[13,21]	[14,23]	[15,25]	[16,27]
6	[6, 6]	[7, 8]	[8,10]	[9,12]	[10,14]	[11,16]	[12,18]	[13,20]	[14,22]	[15,24]	[16,26]	[17,28]
7	[7, 7]	[8, 9]	[9,11]	[10,13]	[11,15]	[12,17]	[13,19]	[14,21]	[15,23]	[16,25]	[17,27]	[18,29]
8	[8, 8]	[9,10]	[10,12]	[11,14]	[12,16]	[13,18]	[14,20]	[15,22]	[16,24]	[17,26]	[18,28]	[19,30]
9	[9, 9]	[10,11]	[11,13]	[12,15]	[13,17]	[14,19]	[15,21]	[16,23]	[17,25]	[18,27]	[19,29]	[20,31]
10	[10,10]	[11,12]	[12,14]	[13,16]	[14,18]	[15,20]	[16,22]	[17,24]	[18,26]	[19,28]	[20,30]	[21,32]
11	[11,11]	[12,13]	[13,15]	[14,17]	[15,19]	[16,21]	[17,23]	[18,25]	[19,27]	[20,29]	[21,31]	[22,33]

Table 3.2. Number of atoms inside the volume of an octahedral fcc(n, k')$_o$ NP, $N_{vol}(n, k')_o$, (volume count) as defined by (C.17 - 20). For the definition of k' see caption of Table 3.1.

List of $N_{vol}(n, k')_o$

$k'\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	1	13	55	147	309	561	923	1415	2057	2869	3871	5083
1	6	38	116	260	490	826	1288	1896	2670	3630	4796	6188
2	19	79	201	405	711	1139	1709	2441	3355	4471	5809	7389
3	44	140	314	586	976	1504	2190	3054	4116	5396	6914	8690
4	85	225	459	807	1289	1925	2735	3739	4957	6409	8115	10095
5	146	338	640	1072	1654	2406	3348	4500	5882	7514	9416	11608
6	231	483	861	1385	2075	2951	4033	5341	6895	8715	10821	13233
7	344	664	1126	1750	2556	3564	4794	6266	8000	10016	12334	14974
8	489	885	1439	2171	3101	4249	5635	7279	9201	11421	13959	16835
9	670	1150	1804	2652	3714	5010	6560	8384	10502	12934	15700	18820
10	891	1463	2225	3197	4399	5851	7573	9585	11907	14559	17561	20933
11	1156	1828	2706	3810	5160	6776	8678	10886	13420	16300	19546	23178

Table 3.3. Number of atoms on the outermost facets of an octahedral fcc(n, k')$_o$ NP, $N_{shell}(n, k')_o$, as defined by (C.21 - 24). For the definition of k' see caption of Table 3.1.

List of $N_{shell}(n, k')_o$

$k'\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	--	12	42	92	162	252	362	492	642	812	1002	1212
1	6	32	78	144	230	336	462	608	774	960	1166	1392
2	18	60	122	204	306	428	570	732	914	1116	1338	1580
3	38	96	174	272	390	528	686	864	1062	1280	1518	1776
4	66	140	234	348	482	636	810	1004	1218	1452	1706	1980
5	102	192	302	432	582	752	942	1152	1382	1632	1902	2192
6	146	252	378	524	690	876	1082	1308	1554	1820	2106	2412
7	198	320	462	624	806	1008	1230	1472	1734	2016	2318	2640
8	258	396	554	732	930	1148	1386	1644	1922	2220	2538	2876
9	326	480	654	848	1062	1296	1550	1824	2118	2432	2766	3120
10	402	572	762	972	1202	1452	1722	2012	2322	2652	3002	3372
11	486	672	878	1104	1350	1616	1902	2208	2534	2880	3246	3632

Table 3.4. Corner distance, $R_c(n, k')_o$, defining the distance from the center of an octahedral fcc(n, k')$_o$ NP to its 24 ($n > 0$, $k' > 0$), 6 ($n = 0$, $k' > 0$), and 12 ($n > 0$, $k' = 0$) corners, respectively. The distances are defined by (C.28). The radii are normalized by the lattice constant a of the fcc lattice. For the definition of k' see caption of Table 3.1.

List of $R_c(n, k')_o / a$

$k'\backslash n$	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.707	1.414	2.121	2.828	3.536	4.243	4.950	5.657	6.364	7.071	7.778
1	0.500	1.118	1.803	2.500	3.202	3.905	4.610	5.315	6.021	6.727	7.433	8.139
2	1.000	1.581	2.236	2.915	3.606	4.301	5.000	5.701	6.403	7.106	7.810	8.515
3	1.500	2.062	2.693	3.354	4.031	4.717	5.408	6.103	6.801	7.500	8.201	8.902
4	2.000	2.550	3.162	3.808	4.472	5.148	5.831	6.519	7.211	7.906	8.602	9.301
5	2.500	3.041	3.640	4.272	4.924	5.590	6.265	6.946	7.632	8.322	9.014	9.708
6	3.000	3.536	4.123	4.743	5.385	6.042	6.708	7.382	8.062	8.746	9.434	10.124
7	3.500	4.031	4.610	5.220	5.852	6.500	7.159	7.826	8.500	9.179	9.862	10.548
8	4.000	4.528	5.099	5.701	6.325	6.964	7.616	8.276	8.944	9.618	10.296	10.977
9	4.500	5.025	5.590	6.185	6.801	7.433	8.078	8.732	9.394	10.062	10.735	11.413
10	5.000	5.523	6.083	6.671	7.280	7.906	8.544	9.192	9.849	10.512	11.180	11.853
11	5.500	6.021	6.576	7.159	7.762	8.382	9.014	9.657	10.308	10.966	11.630	12.298

S.3.3b. Cuboctahedral fcc Nanoparticles, Truncated Cubic Type

Table 3.5. Notation of a non-generic cuboctahedral NP fcc[N, K], fcc(n, k) for given n, k according to $2N = n + k$, $2K = 3n + k$. Structure parameters N, K describe the two generic envelope NPs, cubic fcc[N, 0], fcc[N, 1] and octahedral sc(0, K], sc(1, K] by polyhedral diameters, see Sec. C.3. In contrast, n, k characterize the deviation of the cuboctahedral NP fcc[N, M] from its generic envelope NPs.

For fcc[N, K] NPs of the cubic type, i.e. if $2N \leq K \leq 3N$, $n \geq k$, it is meaningful to use an auxiliary index n' with $n' = (n - k)/2$ resulting in a notation fcc(n', k)$_c$, see Sec. C.3, and yielding

$$[N, K]: \quad N = n' + k, \quad K = 3n' + 2k$$

List of [N, K]

k\n'	0	1	2	3	4	5	6	7	8	9	10	11
0	[0, 0]	[1, 3]	[2, 6]	[3, 9]	[4,12]	[5,15]	[6,18]	[7,21]	[8,24]	[9,27]	[10,30]	[11,33]
1	[1, 2]	[2, 5]	[3, 8]	[4,11]	[5,14]	[6,17]	[7,20]	[8,23]	[9,26]	[10,29]	[11,32]	[12,35]
2	[2, 4]	[3, 7]	[4,10]	[5,13]	[6,16]	[7,19]	[8,22]	[9,25]	[10,28]	[11,31]	[12,34]	[13,37]
3	[3, 6]	[4, 9]	[5,12]	[6,15]	[7,18]	[8,21]	[9,24]	[10,27]	[11,30]	[12,33]	[13,36]	[14,39]
4	[4, 8]	[5,11]	[6,14]	[7,17]	[8,20]	[9,23]	[10,26]	[11,29]	[12,32]	[13,35]	[14,38]	[15,41]
5	[5,10]	[6,13]	[7,16]	[8,19]	[9,22]	[10,25]	[11,28]	[12,31]	[13,34]	[14,37]	[15,40]	[16,43]
6	[6,12]	[7,15]	[8,18]	[9,21]	[10,24]	[11,27]	[12,30]	[13,33]	[14,36]	[15,39]	[16,42]	[17,45]
7	[7,14]	[8,17]	[9,20]	[10,23]	[11,26]	[12,29]	[13,32]	[14,35]	[15,38]	[16,41]	[17,44]	[18,47]
8	[8,16]	[9,19]	[10,22]	[11,25]	[12,28]	[13,31]	[14,34]	[15,37]	[16,40]	[17,43]	[18,46]	[19,49]
9	[9,18]	[10,21]	[11,24]	[12,27]	[13,30]	[14,33]	[15,36]	[16,39]	[17,42]	[18,45]	[19,48]	[20,51]
10	[10,20]	[11,23]	[12,26]	[13,29]	[14,32]	[15,35]	[16,38]	[17,41]	[18,44]	[19,47]	[20,50]	[21,53]
11	[11,22]	[12,25]	[13,28]	[14,31]	[15,34]	[16,37]	[17,40]	[18,43]	[19,46]	[20,49]	[21,52]	[22,55]

Table 3.6. Number of atoms inside the volume of a cubic fcc(n', k)$_c$ NP, $N_{vol}(n', k)_c$, (volume count) as defined by (C.31 - 34). For the definition of n' see caption of Table 3.5.

List of $N_{vol}(n', k)_c$

k\n'	0	1	2	3	4	5	6	7	8	9	10	11
0	1	14	63	172	365	666	1099	1688	2457	3430	4631	6084
1	13	62	171	364	665	1098	1687	2456	3429	4630	6083	7812
2	55	164	357	658	1091	1680	2449	3422	4623	6076	7805	9834
3	147	340	641	1074	1663	2432	3405	4606	6059	7788	9817	12170
4	309	610	1043	1632	2401	3374	4575	6028	7757	9786	12139	14840
5	561	994	1583	2352	3325	4526	5979	7708	9737	12090	14791	17864
6	923	1512	2281	3254	4455	5908	7637	9666	12019	14720	17793	21262
7	1415	2184	3157	4358	5811	7540	9569	11922	14623	17696	21165	25054
8	2057	3030	4231	5684	7413	9442	11795	14496	17569	21038	24927	29260
9	2869	4070	5523	7252	9281	11634	14335	17408	20877	24766	29099	33900
10	3871	5324	7053	9082	11435	14136	17209	20678	24567	28900	33701	38994
11	5083	6812	8841	11194	13895	16968	20437	24326	28659	33460	38753	44562

Table 3.7. Number of atoms on the outermost facets of a cubic fcc(n', k)$_c$ NP, $N_{shell}(n', k)_c$, (facet count) as defined by (C.35 - 38). For the definition of n' see caption of Table 3.5.

List of $N_{shell}(n', k)_c$

k\n'	0	1	2	3	4	5	6	7	8	9	10	11
0	--	14	50	110	194	302	434	590	770	974	1202	1454
1	12	48	108	192	300	432	588	768	972	1200	1452	1728
2	42	102	186	294	426	582	762	966	1194	1446	1722	2022
3	92	176	284	416	572	752	956	1184	1436	1712	2012	2336
4	162	270	402	558	738	942	1170	1422	1698	1998	2322	2670
5	252	384	540	720	924	1152	1404	1680	1980	2304	2652	3024
6	362	518	698	902	1130	1382	1658	1958	2282	2630	3002	3398
7	492	672	876	1104	1356	1632	1932	2256	2604	2976	3372	3792
8	642	846	1074	1326	1602	1902	2226	2574	2946	3342	3762	4206
9	812	1040	1292	1568	1868	2192	2540	2912	3308	3728	4172	4640
10	1002	1254	1530	1830	2154	2502	2874	3270	3690	4134	4602	5094
11	1212	1488	1788	2112	2460	2832	3228	3648	4092	4560	5052	5568

Table 3.8. Corner distance, $R_c(n', k)_c$, defining the distance from the center of a cubic fcc(n', k)$_c$ NP to its 24 ($n' > 0$, $k > 0$), 12 ($n' = 0$, $k > 0$), and 8 ($n' > 0$, $k = 0$) corners, respectively. The distances are defined by (C.42) and all radii are normalized by the lattice constant a of the fcc lattice. For the definition of n' see caption of Table 3.5.

List of $R_c(n', k)_c / a$

k\n'	0	1	2	3	4	5	6	7	8	9	10	11
0	0.000	0.866	1.732	2.598	3.464	4.330	5.196	6.062	6.928	7.794	8.660	9.526
1	0.707	1.500	2.345	3.202	4.062	4.924	5.788	6.652	7.517	8.382	9.247	10.112
2	1.414	2.179	3.000	3.841	4.690	5.545	6.403	7.263	8.124	8.986	9.849	10.712
3	2.121	2.872	3.674	4.500	5.339	6.185	7.036	7.890	8.746	9.605	10.464	11.325
4	2.828	3.571	4.359	5.172	6.000	6.837	7.681	8.529	9.381	10.235	11.091	11.948
5	3.536	4.272	5.050	5.852	6.671	7.500	8.337	9.179	10.025	10.874	11.726	12.580
6	4.243	4.975	5.745	6.538	7.348	8.170	9.000	9.836	10.677	11.522	12.369	13.219
7	4.950	5.679	6.442	7.228	8.031	8.846	9.670	10.500	11.336	12.176	13.019	13.865
8	5.657	6.384	7.141	7.921	8.718	9.526	10.344	11.169	12.000	12.835	13.675	14.517
9	6.364	7.089	7.842	8.617	9.407	10.210	11.023	11.843	12.669	13.500	14.335	15.174
10	7.071	7.794	8.544	9.314	10.100	10.897	11.705	12.520	13.342	14.169	15.000	15.835
11	7.778	8.500	9.247	10.012	10.794	11.587	12.390	13.200	14.018	14.841	15.668	16.500