Appendices
Appendix A
Analysis tools

We introduce the measures that are being used extensively throughout the thesis. Standard measures such as gyration tensor, radial distribution function, velocity autocorrelation function, and mean squared displacement are mentioned from the practice point of view. We also mention the procedure of applying the shape matching order parameter. The details in these analysis tools can easily be found from molecular simulation textbooks and the literature.

A.1 Standard measures

A.1.1 Clustering

In assembled structures such as body-centered cubic micelles, hexagonally packed cylinders or lamellar phases, it is desired to identify separated clusters of nanoparticles (NPs) from which local structural properties, for example, the number of NPs per cluster, or the cluster geometry, center of mass, chirality and helicity, can be extracted. A cluster is defined by a cutoff distance within which the NPs (and their constituent beads) are adjacent neighbors. Given the Cartesian coordinates of the beads under consideration (e.g. of a specific type or in a specific region of the box), the naive clustering algorithm implemented in this thesis involves a recursive function which loops through the neighbors of every bead and adds the beads to the current cluster. Once counted to a cluster, the beads are considered visited. The recursive function returns when all the beads are visited. Note that the beads in a cluster should be sorted by their index to ensure that the beads belonging to an NP are consecutive. In certain cases, the NPs in clusters should also be sorted by their distance to a fixed location in space (e.g. for calculating the helicity parameter of a chain-like cluster). More efficient algorithms (e.g. the disjoint set algorithm) should be implemented if clustering is required frequently during a simulation.
A.1.2 Gyration tensor

Given a cluster of particles with their Cartesian coordinates, the gyration tensor describes the geometrical distribution of the particles with respect to the cluster geometrical center. The gyration tensor is a 3-by-3 matrix of which each element is defined as:

\[ S_{ij} = \frac{1}{N} \sum_{k=1}^{N} (r_{i}^{(k)} - r_{c}^{(k)}) (r_{j}^{(k)} - r_{c}^{(k)}) \]  

(A.1)

where \( i, j = 1, 2, 3; N \) is the number of particles in the cluster; \( r^{(k)} \) and \( r^{C} \) are the particle position and cluster geometrical center, respectively.

The eigenvalues obtained from diagonalizing the gyration tensor reveal the overall shape of the cluster and the corresponding eigenvectors are the major axes. For example, if three eigenvalues are comparable, the cluster has a spherical shape; else if two comparable eigenvalues are much greater than the third, the cluster has a cylindrical shape. To quantify how spherical the cluster is, the asphericity parameter is then defined based on the eigenvalues of the gyration tensor:

\[ A_S = \frac{1}{d-1} \sum_{i>j}^{d} \left( R_i^2 - R_j^2 \right) \left( \sum_{i=1}^{d} R_i^2 \right)^2 \]  

(A.3)

where \( d \) is the dimensionality of the clusters, \( d = 3 \) in most cases; \( R_i^2 \) is the eigenvalues of the gyration tensor. The asphericity parameter varies from zero to unity, corresponds to a spherical shape and a cylindrical shape, respectively. If the cluster is close to spherical, it is common to use the radius of gyration \( R_g \) as an estimate of the radius of the sphere:

\[ R_g^2 = \frac{1}{d} \sum_{i=1}^{d} R_i^2 \]  

(A.4)

A.1.3 Radial distribution function

The radial distribution function (RDF), or pair correlation function, \( g_2(r) \), of a system gives the probability of observing two particles \( i \) and \( j \) separated by a distance \( r \). The probability is usually normalized to the corresponding number density of an ideal gas at the same thermodynamic condition. Given the particles’ position \( r^N \), the radial distribution function
at a separation $r$ is defined as:

$$g(r) = \frac{1}{\rho} \sum_{i=1}^{N} \sum_{j=1}^{N} \delta(||r_i - r_j|| - r)$$  \hspace{1cm} (A.5)

where $\rho = N/V$, $N$ is the total number of particles of interest, $V$ is the system volume, $\delta(\cdot)$ is the delta function, and $||.||$ is the norm L2 operator giving the distance between two particles. Note that when periodic boundary conditions are applied, $g(r)$ is only meaningful when plotted for $r \leq L/2$, where $L$ is the smallest box dimension. RDF provides the isotropic structural information of the system. For example, the distance corresponds to first peak indicates the nearest neighbor shell, to the second peak the next-nearest shell, and so forth. The RDF of a gas state does not have more than one small peak while that of a liquid state may have three distinct peaks. The RDF of a crystal exhibits numerous peaks separated by empty shells (Figure A.1).

![Figure A.1](image)

**Figure A.1** Radial distribution function of a HCP lattice.

### A.1.4 Bond order diagram

The bond order diagram (BOD) shows the local orientational ordering of a structure surrounding any given particle within some distance $r$ or within a certain shell $[r_{\text{min}}; r_{\text{max}}]$. Since the local ordering in the first neighbor shell is often characteristic of the whole system, $r$ is chosen to be the distance corresponding to the first peak in the radial distribution function.
Consider a system of \(N\) beads, for every particle, we loop through all of its neighbors, calculate the normalized displacement vector from the neighbor to the central particle and place this vector at some fixed origin. Figure A.2 shows an example of a BOD for the square grid structure formed by laterally tethered rods calculated from the center of mass of the rods within the shell of \([4.0\sigma;5.0\sigma]\), corresponding to the spacing of the grid (see Section 6.1). The crowded regions indicate the relative position of the neighbors of each rod presumably placed at the center.

The bond order diagram is often used as a fingerprint for characterizing local structures and as an input for the Fourier shape descriptor in the shape matching library discussed below.

\[ C(\tau) = \frac{1}{N} \sum_{i=1}^{N} \frac{\langle \mathbf{v}_i(t_0 + \tau) \cdot \mathbf{v}_i(t_0) \rangle_{t_0}}{\langle \mathbf{v}_i(t_0) \cdot \mathbf{v}_i(t_0) \rangle_{t_0}} \quad (A.6) \]

Figure A.2  Bond order diagram of a square grid structure.

### A.1.5 Velocity autocorrelation function

The velocity autocorrelation function (VACF) is defined as:

The VACF shows how fast a system in equilibrium relaxes, or equivalently, how the dynamics of the system becomes uncorrelated over time. The relaxation time of the system
can be approximated when $C(\tau)$ decays to zero. Note that $\tau$ is not the actual time step in a simulation but the lag between two samples taken at different time slices. To have a good statistical estimate of $C(\tau)$, the reference snapshots $t_0$ should be independent of each other.

An example of the VACF of an equilibrated system is shown as Figure A.3.

**Figure A.3** Velocity autocorrelation function of an equilibrated Lennard-Jones system.

Assume that we have velocities dumped into 100 data files every 10000 steps, $v_J*.dat$, for example, from $t = 39 \times 10^6$ to $t = 40 \times 10^6$. The time span for $C(\tau)$, or the maximum distance between two time slices, is half of this window, i.e. $\tau = 0 - 5 \times 10^5$. First, we should select the number of reference points $N_{\text{refs}}$ used for the ensemble average. For example, $N_{\text{refs}} = 6$ equally spaced reference points at $t_0 = 390 \times 10^5; 391 \times 10^5; 392 \times 10^5; 393 \times 10^5; 394 \times 10^5$ and $395 \times 10^5$. The bigger $N_{\text{refs}}$ and the more distant between reference points, the better the statistics. Figure A.4 illustrate the reference points and sampling points used in this calculation.

Next, we choose the spaces between the time slices, $\tau$, which can follow a linear or a logarithmic scale. For example, a linear scale gives $\tau = 0; 10000; 20000; \ldots, 5 \times 10^5; 10^4; 2 \times 10^4; 5 \times 10^4; 10^5; 2 \times 10^5; \text{and } 5 \times 10^5$. The minimum nonzero value of $\tau$ is the interval between two data files, and the maximum is the time span. This means, for example, with the linear scale above, we are using the velocities at $t = 39210000; 3920000; 39230000; \ldots$ to compute against the velocity at $t_0 = 392 \times 10^5$.

### A.1.6 Mean squared displacement

The mean squared displacement (MSD) is defined as:

$$\langle r^2(\tau) \rangle = \frac{1}{N} \sum_{i=1}^{N} \| r_i(t_0 + \tau) - r_i(t_0) \|_{t_0}$$  \hspace{1cm} (A.7)

The MSD gives the mobility of the system at a given state point. It essentially is the average distance that a given particle travels after time $\tau$. The slope of the MSD plotted ver-
sus time at large $\tau$ giving the self-diffusion coefficient, $D$, according to Einstein’s equation: 
$$\lim_{n \to \infty} \langle r^2(\tau) \rangle = 2dD\tau$$
where $d$ is the system dimensionality. An example of the MSD plot is shown in Figure A.5. At high temperature, the system is diffusive indicated by the positive slope of the MSD at large time intervals. As temperature is decreased, the particles start crystallizing and the slope of the MSD becomes zero at large time intervals.

The calculation of MSD is similar to that of VACF as described above, which involves comparing the particle positions at different states against a reference point, and averaging over several reference points. For example, we want to plot MSD for $\tau = 0 - 10^4$, with the interval of 200, meaning that there would be 50 points in the MSD plot. Assume that we have dumped out atom positions with images included into files at time steps: 11000100; 11000200; 11000300;.. In order to compute the MSD at $\tau$, we need to pick a number of snapshot pairs, calculate the distance between them, and average over the number of pairs. The number of pairs is sometimes called the number of windows, or the number of origins, or reference states. The average is performed over the number of windows. Say, for MSD($\tau = 500$), with 10 windows, we pick 50 snapshot pairs at (11000100; 11000600), (11000300; 11000800), (11000600; 11001100), etc. For each pair, we calculate square
displacement of individual particles and average over all the particles:

$$\frac{1}{N} \sum_{i=1}^{N} \| \mathbf{r}_i(t_0 + \tau) - \mathbf{r}_i(t_0) \|$$  \hspace{1cm} (A.8)

and then average the sum over the number of pairs. Note that we can change the distance between the origins, in this case, 300 to ensure that the reference points are uncorrelated for a good statistics; or choose $\tau$ for MSD from a logarithmic scale rather than a linear scale. Note that to exclude the translational motion of the whole structure from MSD, the center of mass of the system should be kept fixed; or the total momentum should be zero.

**A.2 Shape matching order parameters**

Shape matching order parameter is a generic order parameter that can be applied a wide range of structural characterization. The order parameter is a measure of the degree of the similarity between a sample structure to a reference one through a shape descriptor.
The shape descriptor is essentially an array of information that uniquely characterizes the reference structure, for example, the Cartesian coordinates of the atoms, the peak locations in the diffraction pattern, or the coefficients of the spherical harmonics expansion. Although bearing the term “shape matching”, the order parameter can be extended to incorporate arbitrary aspects other than just geometry-related information. By definition, the difference between the shape descriptor of the sample structure and that of the reference structure, often transformed into a scalar value, gives the matching between these two structures. The difference is often normalized between zero and unity, corresponding to an uncorrelated and a perfect match, respectively. Further detailed explanation of the shape matching order parameter and its applications is given in Reference [221].

In this thesis, we use SMAC (Shape Matching Analysis Code), a open-source C++ library developed by Keys et al. [221], to calculate the shape matching order parameter based on a shape descriptor. The library is available for download in the Glotzilla package. Unlike conventional order parameters characterizing helicity, asphericity and chirality that requires particular mathematical formulation, the application of shape matching order parameters is more generic and flexible. The general procedure is as follows:

**Choose a reference structure**  The reference structure can be either an ideal structure from other database or the final structure which has the desirable properties.

**Plot the radial distribution function for the particles of interest for the reference structure**  The peaks in the RDF plot indicate the location of the shells in which most of the neighbors of a particle in the structure locate. Normally, the first peak is the most important because the interaction is short-ranged in our system and almost negligible to the next-nearest neighbor shell. Exceptions are hierarchically assembled structures formed by a bilayer sheet in Chapter 5.

**Plot the bond order diagram at the vicinity of the shells**  Since the bond order diagram shows the orientational ordering of the neighbors relative to the central particle, we can choose the shells that are characteristic of the reference structure.

**Use the location of the shells as input for the shape descriptor**  When the shells of interest are not spatially adjacent to each other, the particles in the intermediate shells can be disregarded. Multiple choices of the shape descriptor are available in SMAC.
Calculate the scalar metric of the shape descriptor of the reference structure and sample structures

**Calculate the difference between the shape descriptors**  By default, a shape matching order parameter equal to unity corresponds to a perfect match. Since the most uncorrelated match can still have a nonzero matching value, the order parameter should be scaled between unity and the uncorrelated matching to show a good distinction between two extremes. Certainly, the choice of the most uncorrelated is up to the users.

The users need to write a C++ driver program to call these functions using the built-in data structures such as the Fourier shape descriptor, particle coordinates and simulation box data. To compile the program, the compiler (and linker) should be provided with the path to the header files and to the SMAC library. Documentation and examples can be obtained by contacting Glotzer group at http://www.engin.umich.edu/dept/che/research/glotzer/.
Appendix B

Preliminary simulations of reconfigurable and patchy particles

In this appendix, we present our preliminary results on lock-and-key colloidal particles and patchy particles. We show that the reconfigurability of the lock-and-key particles, represented by the mobility of the "lock" particles around the central "key" particle, plays an important role in stabilizing ordered structures other than triangular lattices. We also demonstrate that patchy particles with linear patches self-assemble into helices with a unique handedness. The geometry of the helices are shown to be dependent upon the arrangement of the patches and particle diameter. Though preliminary, our results serve as proof-of-concept for designing complex structures via novel building blocks with reconfigurability and with anisotropic interactions. Our future work would be to further characterize the thermodynamic stability of these structures and to have better statistics for the present results.

B.1 Lock-and-key colloidal particles

B.1.1 Introduction

Lock and key colloidal particles result from the depletion force between colloidal particles with and without dimples, namely, the locks and keys, respectively[3]. The lock-and-key binding results from the entropic gain of depletant molecules escaping from the dimples, causing an effective pulling on the keys towards the dimples. While the binding energy between the locks and the key is strong, in the order of $10k_BT$, the locks are able to rotate around the key, allowing for a unique reconfigurability within the building blocks, which is absent in rigid particles. Additionally, the overlapping between the locks and the key distinguish a system of these particles with that of a mixture of spheres with different sizes.
These features coupled with a plenty of parameters such as the number of locks per key, the center-center distance between the key and the locks, the lock and key size ratio, the confinement condition and the lock mobility relative to the key suggest that these colloidal building blocks are likely to give rise to novel assembled structures. Here we resort to computer simulations to investigate the assembled structures following the parameter axes in Figure B.1. We show that crystalline structures such as HCP or rhombic packing can form within some range of the size ratio and bond length. The constraint and stoichiometry between the locks and keys gives rise to the formation of degenerate crystalline structures of the keys. Also, the confinement in a quasi-3D space contributes to the formation of several unprecedented structures for four-lock particles. The simulation results serve to inspire further experimental study and fabrication of these interesting nanoscale building blocks. This work is conducted in collaboration with Pine’s group, and the results presented here should be considered a preliminary study as proof-of-principle.

Figure B.1  Parameters that influence the self assembly of lock and key colloidal particles
B.1.2 Model and simulation method

Model

Colloidal particles are hundreds of nanometers in size. The key particles are spherical in shape, while the lock particles resemble a pac-man with a curved mouth. The keys and the locks do not directly interact with each other in a pure solvent. When tiny polymers are introduced into the solvent, these polymer molecules attempt to escape from the gap between close colloidal particles to gain more entropy, causing a pressure drop in the gap as compared to the pressure in the bulk. This pressure drop serves as a net ”attractive force” pulling two colloidal particles close together. That ”attractive force” is called the depletion force\[51\].

The depletion force induced when the key comes close to the mouth of the lock is much bigger than when the key comes close to any other (convex) part of the lock (partly because the polymers gain more entropy by escaping from the mouth), $10k_B T$ vs $k_B T$. As a result, when the key fits into the mouth, the key and the lock are ”permanently bonded” at the given temperature. The maximum number of locks per key is constrained by hard-sphere geometry, i.e. the lock/key size ratio and the mouth size. The locks are able to rotate around the key.

We consider several scenarios to model lock and key particles depending on the lock mobility and confinement considerations as follow:

Table B.1 Assembled structures formed with different rod lengths and the dimensionality of the periodicity of the structures.

<table>
<thead>
<tr>
<th>2D particles</th>
<th>The locks are bonded to the key by stiff harmonic springs in the non-rigid model or the bond length is constrained by using the SHAKE algorithm in the rigid model.</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D rigid particles</td>
<td>Every particle is treated as a rigid body.</td>
</tr>
<tr>
<td>Quasi-3D particles</td>
<td>The locks are bonded to the key by stiff harmonic springs in the non-rigid model, or the whole particle is treated as a rigid body in the rigid model. However, the keys are constrained to move on a plane while the keys are allowed to rotate out of the plane.</td>
</tr>
<tr>
<td>3D particles</td>
<td>Non-rigid or rigid particles are allowed to move in 3-D space.</td>
</tr>
</tbody>
</table>

According to experiments, the size ratio between the key and the lock is approximately $D_K/D_L = 0.75$. We choose the key diameter to be $D_K = 1.0\sigma$, the lock diameter is the $D_L = D_K/0.75 = 1.33\sigma$. We also investigate different values of the size ratio in the range of 1.2-1.75. The distance between the lock and the key within a pacman $d_{LK}$ is held by a stiff
string with the spring constant of $k = 3000$. By choosing different spring natural lengths $R_0$, we can adjust $d_{LK}$ within some tolerance effectively similar to using SHAKE. However, at a sufficiently high density, or pressure, the springs can be compressed and the deviation in the bond length becomes greater as compared to using SHAKE.

The non-bonded interaction between the locks and keys are short-ranged as compared to their diameter. We use the Lennard-Jones 12-6 potential truncated and shifted to zero with different $\sigma$ and $\delta$ as follow:

$$U_{LJ-shifted}(r) = \begin{cases} 
4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r-\delta} \right)^6 \right], & r \leq r_C + \delta \\
0, & r > r_C + \delta
\end{cases} \quad (B.1)$$

where $\delta = (D_1 + D_2)/2 - \sigma$, $D_1$ and $D_2$ are the lock and key diameters, respectively.

We shift the potential towards the particle surface and use a value of $\sigma_{LJ}$ much smaller than the particle diameter to capture the short range interaction between colloidal particles. For example, in Figure B.2 $\sigma_{LJ} = 0.1\sigma$, $D_1 = 1.0\sigma$ and $D_2 = 1.33\sigma$. At high pressure, the particles interact via the WCA potential with $r_C = 2^{1/6} \sigma_{LJ} = 0.1122\sigma$. At low density, the depletion attraction between the locks and keys is modeled by the LJ potential with $r_C = 2.5\sigma_{LJ} = 0.25\sigma$. The depletion attraction between the locks is in the order of $k_BT$.

![Figure B.2](image)

**Figure B.2** Shifted 12-6 Lennard-Jones potential truncated at $r_C = 2^{1/6} \sigma_{LJ} = 0.1122\sigma$ to capture the short-ranged repulsion between particles.
Simulation method

We use Brownian dynamics to simulate systems of constant number of colloidal particles at constant temperature and volume, i.e. canonical ensemble. The systems are initialized at athermal conditions, i.e. all interactions are purely repulsive, for being well-mixed. For high pressure simulations, the box is gradually compressed or rescaled until crystallization is observed. To relieve defects, the box might be slightly expanded in a short time period, and then re-compressed. For low pressure simulations, the box is rescaled until the packing density reaches 0.3-0.4 to facilitate the aggregation of the particles.

B.1.3 Results and discussion

We focus on the parameters that are readily tunable in experiments in Pine’s group at the time of this thesis being written. The parameters of interest are the lock-key distance (bond length), lock-key size ratio, lock mobility, number of locks per key, and spatial confinement as shown in Figure B.1. We investigate the assembly at high density and low density limits and show that the mobility of the locks plays a more influential role in the packing pattern of resulting structures at low pressure than at high pressure.

High density limit

Lock-key distance and size ratio Considering the two-lock particles, we investigate the size ratios \( D_L/D_K = 1.2; 1.33; 1.5 \) and 1.75, which are in the range of the particles in practice. For each value of \( D_L/D_K \), we vary the center-center distance between the lock and the key in the range of \((D_L/2; (D_L + D_K)/2)\). The lower bound corresponds to the case where two locks touch each other, and the upper bound to the case where the lock touch the key. \( D_K = 1.0\sigma \) for all cases. The structures under comparison are obtained at a packing density of 0.85.

We observe that the locks (yellow) can form a hexagonal close packing (HCP) structure for a certain range of \( d_{LK} \) and \( r \). Representative snapshots in Figure B.4 compare a good HCP structure (Figure B.3(a)) versus a disordered structure (Figure B.3(b)) of the locks at \( D_L/D_K = 1.33 \). The peaks in the diffraction pattern (Figure B.4(a), middle) are indicative of the six fold symmetry of the HCP structure of the locks. The keys (blue) are located on a degenerate kagome lattice due to the constraint: every key has two and only two locks. The diffraction pattern of the keys (Figure B.3(a), bottom) shows the peaks corresponding to the underlying HCP lattice formed by the locks. The noisy parts surrounding the peaks
Figure B.3 Structures formed by 2-lock particles with (a) $d_{LK} = 0.75\sigma$ and (b) $d_{LK} = 1.0\sigma$ for the size ratio $D_L/D_K = 1.33$. Top: snapshot with the keys in blue and locks in yellow. Middle: only the locks are visualized. Bottom: only the keys are visualized. Insets are the diffraction patterns.

correspond to the disordered arrangement of the keys. On the contrary, for the disordered structure neither the diffraction pattern of the locks or that of the keys shows any peak (Figure B.3(b)).

The distribution of the bond angle shown in Figure B.4 demonstrates the conformation of individual particles ($D_L/D_K = 1.33$) within the final structures. In a HCP structure ($d_{LK} = 0.7\sigma$), the two-lock particles adopt a uniform linear geometry with most of the angles being $180^\circ$. As the bond length increases ($d_{LK} = 0.9\sigma$ and $1.1\sigma$) the distribution is shifted towards smaller angles and becomes more polydisperse, corresponding to more disordered structures. For $d_{LK} = 1.1\sigma$, where the depth of the locks is the most shallow, the peak around $\theta = 76^\circ$ indicates that $\approx 20\%$ of the particles have adopt a V shape with two locks touching each other, which makes them incompatible with the packing into a HCP structure.

**Lock mobility** The mobility of the locks of a particle can be characterized by the free volume accessible by the locks on the key surface. For a given size ratio $D_L/D_K$ the greater
Figure B.4  Distributions of the bond angle of individual two-lock 2D particles ($D_L/D_K = 1.33$) with different bond lengths.

the distance $d_{LK}$, the greater the lock mobility because the locks have more accessible volume on the key surface. We choose the best HCP structure of the locks for a given value of $D_L/D_K$ as the reference state and calculate the shape matching order parameter of the final structures obtained for each pair of $(D_L/D_K, d_{LK})$. As can be seen in Figure B.5(a), the optimal range to observe the HCP structure is shifted to higher values of $d_{LK}$ as the size ratio increases. That range of $d_{LK}$ is equivalent to the optimal range of the lock mobility for the stabilization of the HCP structures at a given size ratio. Beyond that range of the lock mobility the particles form a disordered solid.

Another approach to completely remove the lock mobility is to make the particles rigid by fixing the relative position of the locks with respect to the key. We infer from Figure B.4 that in a HCP structure, the particles are most likely to have a linear shape; thus, we consider the case where the locks and key are “frozen” in a linear geometry, making a dumbbell-shaped rigid particle. Figure B.5(b) shows the HCP order parameter for rigid particles as a function of $D_L/D_K$ and $d_{LK}$. Comparing the HCP order parameter in Figure B.5(b) with that in Figure B.5(a), we observe a similar behavior, i.e. there is an optimal range of $d_{LK}$ for each value of size ratio $D_L/D_K$ in which the locks form an ordered HCP structure. The range is also broadened to higher values of $d_{LK}$ for a given value of $D_L/D_K$. For example, for $D_L/D_K = 1.33$, the rigid particles assemble into a HCP structure as $d_{LK}$ does not exceed $0.95\sigma$; meanwhile, the lock mobile particles can retain the HCP structure.
Figure B.5  HCP shape matching order parameter with different lock-key size ratio \((D_L/D_K)\) and bond length \(d_{LK}\). Each curve is obtained by averaging across several independent runs. Error bars are smaller than the marker size. (a) Locks are able to move around the key. (b) Locks and key within a particle are rigid into a linear geometry. up to \(d_{LK} = 0.8\sigma\).

**Number of locks per key**  In addition to two-lock particles, we consider particles with three and four locks, also varying the bond length and size ratio. Similar to two-lock particles, the locks of these particles can form crystalline structures within an optimal range of lock-key bond length and size ratio. Beyond the optimal range the assembled structure do not exhibit any long range order. In their crystalline states, the locks of three- and four-lock particles assemble into a HCP lattice and a rhombic lattice, respectively. For three-lock particles the bright peaks in the diffraction pattern of the keys in the crystalline state indicates that the keys are constrained within the HCP lattice of the locks (Figure B.6(a)). The noise surrounding the peaks shows their local disorder. The dark lines correspond to the space occupied by the locks that is inaccessible to the keys.

The keys of four-lock particles are restricted in a rhombic lattice of the locks as indicated by the peaks in the diffraction pattern (Figure B.6(b)). The snapshot shows the presence of several grain boundaries caused by the finite relaxation time in our simulations. The orientation of the grains is shown in the bright stripes in the diffraction pattern. We note that unlike for two- and three-lock particles, the locks of four-lock particles compromise between forming a rhombic lattice and forming a triangular lattice. The former results from intra-particle constraints, i.e. the square shape of the particles; the latter results from inter-particle constraints, i.e. the locks from neighboring particles always tend to pack into a HCP lattice.
Spatial confinement We extend the spatial confinement from 2-D to quasi-3D, where the keys are confined in the x-y plane and the locks able to rotate out-of-the plane. This confinement is to reproduce the experimental condition where the particles can move within a thin film or on a substrate without diffusing to the z direction. We choose to show the results of the three-lock particles; the simulations for two- and four-lock particles are underway. We vary the bond length and size ratio and observe the formation of different packing patterns at the packing density of 0.7.

As can be seen in Figure B.7, there is a disordered-ordered transition in the assembled structure of the locks as the bond length decreases. For $D_L/D_K = 1.33$ the transition occurs between $d_{LK} = 0.95\sigma$ and $d_{LK} = 1.0\sigma$. For smaller bond lengths, the crystalline structures exhibit a four-fold symmetry at $d_{LK} = 0.95$ and $d_{LK} = 0.9\sigma$.

We compare the crystalline structures formed at $d_{LK} = 0.8\sigma$ and $d_{LK} = 0.9\sigma$ in Figure B.8. As indicated by the bond order diagram measure for individual particles, the particles adopt a tri-star shape for $d_{LK} = 0.8\sigma$ (Figure B.8(a)) and a T shape for $d_{LK} = 0.9\sigma$ (Figure B.8(b)). The difference in the particle conformation leads to different packing patterns as shown in Figure B.7. The star shape particles tilt with respect to the x-y plane and stack into rows to have an efficient packing.
Figure B.7  Assembled structures formed by three-lock particles with the keys constrained on the x-y plane with different bond lengths for the size ratio of $D_L/D_K = 1.33$.

B.1.4 Low density limit

We investigate the self-assembly of two- and three- lock particles in 2-D space at the low density ($\phi < 0.1$). The motivation for studying this limit is to phase out the effects of high pressure on the lock mobility. The aggregation of the particles is induced at $T^* = 0.25$ in a simulation space sufficiently large to avoid periodic boundary effects. We found that the size ratio, bond length and lock mobility altogether give rise to unique tiling patterns that are not observed for rigid particles.
Figure B.8  Four-fold symmetry structure formed by quasi-3D three-lock particles. (a) \(d_{LK} = 0.8\sigma; D_L/D_K = 1.33\) and (b) \(d_{LK} = 0.9\sigma; D_L/D_K = 1.33\). Left: Side-view of a portion of the assembled structure. Right: Bond order diagram of individual particles.

Two-lock particles

As shown in Figure B.9, the locks of two-lock particles form a HCP lattice for \(D_L/D_K = 1.75\) or an aperiodic lattice composed of triangles and squares for \(D_L/D_K = 1.5\). For \(D_L/D_K = 1.75\) and \(d_{LK} = 0.9\sigma\) (Figure B.9 left), the locks form a hexagonal lattice at high density similar to that observed at high density (Figure A2.3(a)). The particles also adopt a linear geometry. In this case, the lock mobility is small and the HCP lattice is always favored regardless of density.

As the size ratio is decreased to \(D_L/D_K = 1.5\) (Figure B.9 right), the lock mobility is increased, the HCP lattice does not form at low density as observed at high density (Figure B.5(a)). Instead, we found that the locks form a lattice composed of regular triangles and squares. The tiling pattern is a random mixture of the elongated triangular tiling \((3^2.4^2)\) and snub square tiling \((3^2.4.3.4)\). The Bragg peaks in the diffraction pattern of the locks suggests that there is an underlying 12-fold symmetry lattice in the structure. The bond angle distribution further reveals that the particles adopt a 120-degree conformation within the lattice. This is interesting because a small change in the size ratio, hence the lock mobility, could lead to a remarkable change in the packing pattern of the assembled structure.
Figure B.9  Two-lock particles with the bond length of $d_{LK} = 0.9\sigma$ and different values of bond length $D_L/D_K$

Three-lock particles

Figure B.10 shows different assembled structures from three-lock particles with the same size ratio. As the bond length increases, the locks have more mobility on the key surface. For small lock mobility ($d_{LK} = 0.85\sigma$), the locks form a HCP pattern as expected because the particles all have a tri-star conformation. For higher lock mobility ($d_{LK} = 1.0\sigma$), the locks form an ordered lattice of oval-shaped tiles. The oval-shaped tiles are made of the particles in a T-shaped conformation packing side-by-side.

For a greater lock mobility ($d_{LK} = 1.15\sigma$), the locks form an aperiodic ordered lattice composed of triangles, rhombs and pentagons while the keys located at the center of the pentagons, aligning into stripes. The pentagons are coupled into pairs, surrounded by three rhombs and three triangles. The diffraction pattern of the locks indicates a long range ordering despite a non-trivial real-space pattern. Interestingly, within the lattice, the particles adopt a symmetric Y-shaped conformation with two locks touching each other and the third lying on the particle symmetric axis. Again, these results demonstrate that the lock mobility allows for the particles to assemble into structures much more interesting than HCP lattices.
Figure B.10  Three-lock particles with a size ratio of $D_L/D_K = 1.33$ and different values of bond length $d_{LK}$. The lock mobility increases along with the bond length (from left to right).

B.1.5 Conclusion and ongoing work

We have investigated several parameters that strongly influence the self-assembly of lock-and-key particles. The most salient feature of these particles as compared to other previously studied building blocks is the lock mobility, which lends them a unique flexibility to have efficient packing. At high density, the size ratio and bond length play much more significant role than the lock mobility in stabilizing crystalline structures at high pressure or density. However, at low density, the lock mobility becomes more pronounced, allowing the particles adopt conformations that maximize the local packing fraction. As a result, the particles assemble into various structures with tiling patterns that are inaccessible with rigid particles with the same size ratio and bond length. Simulations on the described systems are underway for better statistics. Additionally, further characterization of the aperiodic assembled structures formed by three-lock particles at low density will be the focus of our future study.

B.2 Patchy particles

We aim at engineering helical structures from the self-assembly of spherical patchy particles with two linear patches, intentionally arranged to create a directional lock-and-key interaction between particles. This section presents preliminary results in this direction. Using molecular dynamics, we find that there is an optimal range of the particle size and patch arrangement that maximize the probability of such anisotropic building blocks assembling into helices. Within the optimal range, the assembled helices are shown to match with the
target structure as prescribed by geometry calculations and to be robust with the patch size.
Out of this range, the building blocks are likely to aggregate into rings or random coils. The
aggregation of the patchy particles can be characterized as an equilibrium polymerization as
the monotonous growth of the cluster size and the continuous change in the system potential
energy.

B.2.1 Introduction

The fabrication of next-generation functional materials has been favorable with the avail-
ability of assembling building blocks with diverse shape, size and chemical functionality.
The anisotropy of assembling building blocks in fact can be characterized by a multi-
dimensional parameter space as proposed by Glotzer et al.[25] including aspect ratio,
patchiness, surface quantization, branching and roughness. Along one of these dimen-
sions, the variation in the particle patchiness, or surface coverage, gives rise to a novel
class of assembling building blocks, which are distinguished by their ability to robustly
self-assemble into desired structures with high monodispersity. It is the highly anisotropic,
strongly directional interactions between patches that allow the modified particles to interact
in the same fashion as virus capsid proteins and many biological molecules. With the
rapid progress in synthesis techniques since 1990s such as templating[155][243], colloidal
assembly[244][245] or particle lithography[246], it is now possible to synthesize such
patchy particles with multiple levels of complexity in a large batch volume. Theoretical
models for patchy particles serving as a predictive tool for experiments have also been
constant developed in attempts to understanding the roles of anisotropic interactions,
thermodynamic parameters and patch properties on the particle assembly behaviors. Ex-
amples for such theoretical models include the water-mimicking particles[247][248], stick
hard spheres[235][249][250], bumpy particles with distinguishable atoms[27][251][254],
particles with protein-like interactions[28][29][233][255][260] and density functional theory
models[261][262]. Further details on fabrication methods can be found in a thorough review
performed by Pawar et al.[263]

It has been shown that the self-assembly of patchy particles and their biological analogs
such as virus capsid proteins and surface functional globular proteins depend on a large
number of parameters in addition to thermodynamic variables and solvent conditions. The
particle shape and the patch arrangement, geometry and selectivity are all identified as
important factors that can influence the self-assembly significantly. Using molecular dynam-
ics, Rapaport first showed how patchy particles in a trapezoidal shape easily assemble into
capsid-like structures given that the interactions between the sticky spots follow certain rules
in sequence\textsuperscript{251}. Relaxing those nonphysical rules, Nguyen et al. developed two other shape model patchy particles, both of which spontaneously assemble into capsid structures with different triangulation numbers\textsuperscript{253}. In their work the special particle shape and the patch selectivity are key to the successful formation of capsid-like structures. The patch size and shape are also been shown to have profound effects on the formation of target structures. Wilber et al. studied the assembly of a five-patch particle with protein-like interactions, showing that the optimal patch width for icosahedral clusters results from the competition between energetic and kinetic requirements\textsuperscript{29}. In 2004, Zhang and Glotzer proposed a bumpy particle model made of distinguishable ”atoms”, which allows for capturing the directional interactions between particles with a remarkable flexibility by specifying interactions between patch ”atoms”\textsuperscript{27}. They predicted a wide spectrum of assembled structures by varying the particle shape, patch arrangement, composition and geometry. For example, spherical particles form sheets when the patches are attached around the equator; triangular plates stack into a twisted structure with a linear patch on a face, and stair-case structures with V-shaped patches on two faces. If each linear patch is made of two dislike molecular types, the patches help align binding particles in an energetically favorable configuration. Later, they proposed a stick hard sphere model which assembles into diamond structures, which can be further stabilized by additional ”bond” angle interactions. These inspiring results suggested that linear patches can be judiciously arranged to induce angle constraints on the aggregation of patchy particles. In this contribution, we extend the Zhang and Glotzer’s model and introduce another family of assembled morphologies from patchy particles, helical structures with a uniform chirality. We show that the patchy particles successfully assemble into target helices dictated by the particle size and patch arrangement. By tuning the particle size and patch arrangement, we can drive the assembly of patchy particles from helices to linear chains and closed rings. We also find that the formation of the helices is robust over a considerable range of the patch width, suggesting that the patchy particles are likely to adopt a high propensity to form helices in experiments. The autonomous and precise formation of such helical structures serves to inspire the fabrication of functional nanostructures with unique electronic and optical properties, and more generally, to propose an approach to incorporate directional lock-and-key interactions into isotropic building blocks.
B.2.2 Model and simulation method

Model

We employed a generic coarse-grained model similar to the distinguishable atom model used by Zhang and Glotzer[27]. The patchy particles are treated as rigid bodies that are able to freely move in a three dimensional space. Each spherical patchy particle consists of $N_S$ beads with diameter $\sigma$ on the surface and two linear patches, each of which is composed of $N_F = 6$ beads, with the same diameter $\sigma$, of two molecular types. The arrangement of the linear patches is given by two angles $\phi$ and $\theta$, determined by the particle center and the patch centers in the body-fixed frame. The patch width $W$ and the patch height $\delta$ are defined as illustrated in Figure B.11. Because of symmetry, we show the results for $\theta$ in the range of $[0^\circ; 90^\circ]$ and $\phi$ in the range of $[0^\circ; 180^\circ]$. The assembled structures with the other ranges of these angles are identical but with the opposite handedness.

![Figure B.11](image)

**Figure B.11** Model patchy particle with two linear patches, each consisting of two non-attractive types of molecules (A, B) and (C, D). The top left figure shows the model for $D = 7.0\sigma$. The surface beads (white) are hidden in the bottom left and right images for clarity.

The interactions between the molecules in the patches are specified such that the patchy particles are energetically favored to aggregate into ring structures as indicated in Reference [27]. The obvious advantage of our model is that the anisotropic interaction between patchy particles is inherently incorporated in the linear shape of the attractive patches. As a result, isotropic interactions such as the standard Lennard Jones and Weeks-Chandler-Andersen potentials can be used to represent the attractive or purely repulsive interactions between constituent beads, respectively. Additionally, the coarse graining into bumpy spheres on the surface represents the interactions between actual patchy particles, which is short ranged as compared to the particle diameter. Specifically, the aggregation of the beads from attractive
stripes, i.e. (A; D) and (B; C), is modeled by the 12-6 Lennard-Jones potential truncated and shifted to zero at the cutoff distance of $2.5\sigma$. The interaction between the non-attractive beads (the other pairs) is modeled by the Weeks-Chandler-Andersen potential.

**Simulation method**

Molecular dynamics is used to simulate a system of the model patchy particles in a three dimensional volume. We use the Nose-Hoover thermostat coupled with both the translational and rotational degrees of freedom of the rigid bodies such that our simulations sample the isothermal ensemble. The motion of the rigid particles, which are initialized randomly in the simulation box is achieved using the velocity Verlet algorithm with quaternions with a time step $\Delta t = 0.002\tau$. The number of particles ($N_P$) ranges from 64 to 216 to ascertain that the obtained structures are consistent. For each parameter set, we perform 4-5 independent simulation runs to ascertain that the results are consistent and statistically meaningful. The simulation results were produced using LAMMPS and HOOMD-blue, open-source parallel molecular dynamics codes.

**B.2.3 Results and discussion**

We first determine the temperature $T^*$ below which the particle aggregation occurs. By monitoring the maximum cluster size and system potential energy at different temperatures, we find that the patchy particles assemble into clusters in analogy with equilibrium polymerization rather than a first-order phase transition. We then present the phase behavior of patchy particles with different particle sizes as function of the patch arrangement ($\phi$ and $\theta$) at a sufficiently low temperature. Within the optimal range of $\phi$ and $\theta$, the helix radius and pitch match perfectly with geometrical calculations, indicating that the self-assembly into target helices is well controlled. Additionally, the helices are shown to be robust with respect to a wide range of the patch size.

**Assembly dynamics**

We investigate the dynamics of the self-assembly of patchy particles with different values of $(D/W, \phi, \theta)$. Our results reveal that the aggregation of patchy particles mainly depends on the reduced temperature $T^*$, i.e. the attraction strength $\epsilon$ between the patches and temperature $T$ regardless of the particle size and patch arrangement. The system potential energy $U$ at instantaneous temperatures and upon heating and cooling are shown in Figure B.12(a).
There is neither hysteresis nor discontinuity in $U$ upon heating and cooling, indicating that the aggregation is analogous to equilibrium polymerization, rather than a first-order phase transition. To investigate the assembly dynamics, we start with a small size system of $N_p = 24$ patchy particles with $D/W = 5.0$, $\phi = 30^\circ$ and $\theta = 45^\circ$. The time evolution of the maximum cluster size at different temperatures for that system is shown in Figure B.12(b). For $T^* \geq 0.67$, the particles remain isolated and diffuse throughout the box, as indicated by the maximum cluster size being fluctuating around one and the system potential energy close to zero. The particles aggregate into robust clusters when the attraction strength between patches $T^*$ is less than 0.67. The maximum cluster size increases versus time in a step-wise manner, suggesting that the particles first assemble into small aggregates, which subsequently merge into bigger clusters. The maximum cluster size reaches the total number of particles, indicating that the particles tend to form one big cluster. For a system of 1000 particles at $T^* = 0.25$, the average cluster size increasing (Figure B.12(c)) and the cluster size distribution shifting towards large values over time (Figure 2(d)) indicate that the particle aggregation is not size limiting. Patchy particles with other values of $(D/W, \phi, \theta)$ also exhibit similar dynamic behaviors.

**Energy landscapes**

We investigate the effects of the patch arrangement and article size while fixing the patch size ($W = 1.0\sigma$ and $\delta = 20^\circ$) on the assembled structures. Since the potential energy minimizing configurations are those in which the patches perfectly match each other, corresponding to helical structures for $\theta < 90^\circ$, the emergence of rings and random coils is considered competing morphologies with higher potential energy. The difference in the potential energy between the helices and their competing morphologies, however, becomes negligible when the chain gets longer. As a result, it is more likely to observe rings and coils than helices in certain ranges of $(\phi, \theta)$. In the following, we show the energy landscape in terms of $(\phi, \theta)$ where the structures reported in each color coded region have a frequency of occurrence greater than 60%. In general, the plots show the helical state is surrounded by higher energy barriers marked by rings and coils.

The energy landscape for the particle sizes of $D/W = 4.0$, 5.0, 6.0, 7.0 and 8.0 are obtained at $T^* = 0.25$. For $D/W = 4.0$, in addition to helices, spherical patchy particles may assemble into random coils and rings as by products (Figure B.13). At small $\phi$ and large $\theta$, the patch centers are close to each other and to the particle equator; the particles tend to lock into rings similar to those in Reference [27] (Figure B.13(b)). For larger values of $\phi$, the patches are more separated; and the particles are more likely to aggregate into random
Figure B.12 Assembly dynamics: (a) Per particle system potential energy upon heating and cooling. Error bars are smaller than the markers. (b) Time evolution of the maximum cluster size versus time at different temperatures for a system of 24 particles. (c) Time evolution of the average cluster size for a system of 1000 particles at $T^* = 0.25; 0.67$ and 10.0. (d) The cluster size distribution for a system of 1000 particles at $T^* = 0.25$ as the system evolves.

Coils (Figure B.15c). For small values of $\theta$, the patch centers though close to each other are far from the particle equator, resulting the formation of helices (Figure B.13d)). The comparable helix and coil regions suggest that there would be a competition between these two structures for patchy particles with $D/W = 4.0$.

For $D/W > 4.0$, the landscapes are divided into two regions: rings for $\theta = [60^\circ; 90^\circ]$ and helices for $\theta = [0^\circ; 45^\circ]$ (Figure B.14). Similar to smaller size particles, the bigger particles form rings for $\theta = [60^\circ; 90^\circ]$ when the patches are located close to the particle equator. Random coils only form for $D/W = 5.0$ at high values of $\phi$ and $\theta$ where the patches are far apart. As their size increases, the coil region vanishes; and the particles tend to form either rings or helices. The absence of the coil region for $D/W > 4.0$ indicates that the particle size should exceed a certain threshold to stabilize the formation of helices for a given patch size. However, as the particle size increases, the ring region is also broadened particularly at high
Figure B.13 (a) Energy landscape for patchy particles with $D/W = 4.0$. Rings (R), random coils (C) and helices (H) form depending on the patch arrangement. The legend on the right shows the frequency of occurrence of the helices. Example snapshots: (b) rings formed at ($\phi = 90^\circ; \theta = 0^\circ$) (left) and ($\phi = 120^\circ; \theta = 60^\circ$) (right); (c) a random coil formed at ($\phi = 120^\circ; \theta = 45^\circ$); (d) helices formed at ($\phi = 30^\circ; \theta = 30^\circ$) (left) and formed at ($\phi = 150^\circ; \theta = 0^\circ$) (right).

$\phi$ and $\theta$. This is because the imperfection in the patch aggregation, which is comparable to the helical pitch, allows the two chain ends to lock together. It is important to note that at $T^* = 0.25$, the assembled clusters are highly unlikely to dissolve or re-arrange once formed and thus suffer from kinetic traps. At higher temperatures ($0.25 \leq T^* \leq 0.67$), the helix region will be broadened because the particles are able to re-orient maximize their energetically favorable patch contacts.

The effects of $\theta$ with a given size ratio $D/W$ and $\phi$ on the geometry of the helices are shown in Figure B.15. For $D/W = 5.0$ and $\phi = 120^\circ$, we observe that the helical radius increases with $\theta$ while the helical pitch fluctuates widely during the simulation. The angles used in Figure B.15 are those in the optimal range found in Figure B.14.

Meanwhile, for $D/W = 7.0$ and $\theta = 45^\circ$, the assembled helices are more well controlled by $\phi$. We notice the monotonous increase in the helical radius and pitch as $\phi$ increases from $30^\circ$ to $150^\circ$. Although the helices are also subject to thermal fluctuations, they seem to retain their shape better than varying $\theta$. 

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Figure B.14  Landscapes for different particle sizes (a) $D/W = 5.0$; (b) $D/W = 6.0$; (c) $D/W = 7.0$ and (d) $D/W = 8.0$. Rings (R), random coils (C) and helices (H) form depending on the patch arrangement. The boundaries are drawn to guide the eyes. The legend on the right shows the frequency of occurrence of the helices.

Figure B.15  Helices formed by patchy particles with $D/W = 5.0$ and $\theta = 120^\circ$: (a) $\theta = 0^\circ$; (b) $\theta = 45^\circ$; (c) $\theta = 75^\circ$ and (d) $\theta = 90^\circ$. 
Figure B.16  Helices formed by patchy particles with $\frac{D}{W} = 7.0$ and $\theta = 45^\circ$: (a) $\phi = 30^\circ$; (b) $\phi = 60^\circ$; (c) $\phi = 90^\circ$; (d) $\phi = 120^\circ$; and (e) $\phi = 150^\circ$.

B.2.4 Conclusion and outlook

We have shown that patchy particles with two linear patches arranged in a non-planar fashion self-assemble into helical chains. The directional and selective interaction of the patches resemble the lock-and-key interaction between globular proteins, giving rise to the formation of helices whose the length scale is much greater than the building blocks themselves. The chirality of the building blocks leads to the unique handedness of the helical structures. We find that for a given particle size the helices are most likely to be observed in a certain range of the arrangement, represented by two angles ($\phi$; $\theta$). Meanwhile, rings and random coils are competing kinetically trapped configurations. The focus of future study is to map the energy landscapes for different patch arrangements and particle size, which provide useful information on the robustness of engineering helical structures with a uniform chirality. We expect that this study would inspire the fabrication of such building blocks, aiming at an inorganic analogy of biological supramolecules.
Appendix C

VisualizerX visualization software

C.1 Introduction

We have been developing VisualizerX, a graphical user interface (GUI) software for visualizing 3-D molecular simulation data since 2006. VisualizerX is implemented using Microsoft® Visual C++®, Microsoft® Foundation Classes® (MFC) and OpenGL. The software requires Windows XP or later and at least 512MB RAM. The distribution package consists of the binary executable (VisualizerX.exe, 1.5MB) and MFC and OpenGL dynamic linked libraries (mfc42d.dll, mfco42d.dll, msvcrtd.dll, msvcrtd.dll, msvcp60d.dll, glu32.dll, glut32.dll and opengl32.dll). Trial versions and user manual can be obtained by contacting the author at ndtrung@umich.edu.

In addition to the standard interface of a Windows application, the most powerful feature of VisualizerX is the user-defined template for drawing 3-D particles. Users can declare how to draw individual building blocks from primitive geometries in a text file and apply the template to the XYZ data. VisualizerX can be used with other visualization packages for further analysis. Most of the visual results in this thesis are obtained from VisualizerX.

C.2 Features

VisualizerX reads in the particle XYZ coordinates and shows them on the main window. As of version 1.10.00 VisualizerX offers the following features:

C.2.1 Visualization

- Flexible user-defined building block primitives: cylinders, polygons, polyhedra, spheres with different diameters, lines and more to be added if requested
- Overlay vectors (i.e. dipoles, velocities, accelerations) to individual particles
Figure C.1 VisualizerX 1.10.0 welcome screen

- Multiple views and multiple structures at the same time

C.2.2 Analysis

- Radial distribution function for specified atom types in 2-D and 3-D
- Bond order diagram for specified atom types and ranges
- Diffraction pattern for selected particles
- Filter particles based on region (box or sphere), types and indices
- Interactive manipulation
- Zoom, translate in and out, scaling, camera setup with mouse clicks
- Shift in X-, Y- and Z- directions with periodic boundary conditions
- Materials color can be adjusted interactively
- Special effects: lighting, blending, fogging and outlines
- Replicate selected particles
Figure C.2  Honeycomb structure formed by laterally tethered nanorods. Users can adjust viewing parameters, lighting conditions and materials colors interactively.

Figure C.3  Radial distribution function, bond order diagram and diffraction pattern of a quasicrystalline structure formed by “bumpy” soft tetrahedra. Only centers of mass are visualized. "Bonds" represent distances between particle centers at the first peak of the radial distribution function.
C.2.3 Input/Output

- Support drag-and-drop XYZ-format files directly to the main window
- Support Copy/Paste (Device Independent Bitmap- DIB) images into documents e.g. Microsoft®Office® and Paint®. Note that DIBs in PowerPoint can be saved as high resolution images (up to 300 dpi) with ExportBitmapResolution set in the Windows® registry. Higher DPIs can be achieved by GIMP
- Support streaming from ASCII files which are produced by concatenating multiple .XYZ files for animated visualization and screen-capture software
- Support streaming from standard input
- Support exporting to BMP images
- Support exporting to Encapsulated Post Script (EPS) files

C.3 Future development

In the future, the DCD data format and other image formats such as PNG and JPEG will be supported. Other special effects with lighting and refraction will be implemented. Functionalities can be further added to VisualizerX upon request.
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