disLocate - *Mathematica* Package:

(d)etecting (i)ntermolecular (s)tructure (Locate)d at particle positions

Load the disLocate.m Package into *Mathematica:*

1. Install Package:
Menu Bar > File > Install... > Type [Package] Source: [From File...] Name: [disLocate] > [OK]

Click the Blue Cell and Press the Two Buttons: "Shift" + "Enter"

```
<< disLocate`
disLocateVersion
```

```
1.2017-08-04.thesis
```

Note: Make sure this line produces a version number before continuing

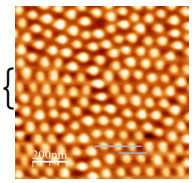
Select and Import the Data Files

2. Run all Examples by clicking:
Menu Bar > Evaluation > Evaluate Entire Notebook

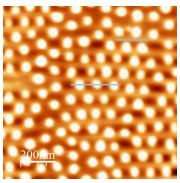
NOTE: Make sure this notebook is in the same directory as the data folder: micelle_data/

```
dir = NotebookDirectory[] <> "micelle_data/";
SetDirectory[dir];
```

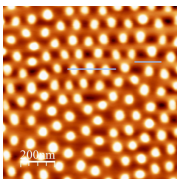
```
images = {
```



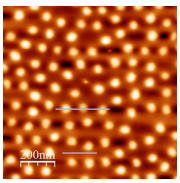

```
,
```




```
,
```




```
,
```




```
};
```

```
xylene2000 =
  Import[dir <> "2000rpm/Result 2000rpm 1um.csv", "CSV"][[2 ;;, 3 ;; 4]];
xylene4000 = Import[dir <> "4000rpm/Result 4000rpm 1um.csv", "CSV"][[
   2 ;;, 3 ;; 4]];
xylene6000 = Import[dir <> "6000rpm/Result 6000rpm 1um.csv", "CSV"][[
   2 ;;, 3 ;; 4]];
xylene8000 = Import[dir <> "8000rpm/Result 8000rpm 1um.csv", "CSV"][[2 ;;, 3 ;; 4]];
```

```
xyXyleneList = {xylene2000, xylene4000, xylene6000, xylene8000};
nameList = {"2000rpm", "4000rpm", "6000rpm", "8000rpm"};
```

Voronoi Tessellations - Area Distributions

In[58]:= **? PlotVoronoiTessellations**

PlotVoronoiTessellations[data2Din_, OptionsPattern[]]:= Returns a Graphics of the VoronoiCells[]
that has been colour coded to associate disorder metrics to the planar arrangements.
OptionsPattern=(type→ToString[vor],symmetry→6,cells→{},points→True,scalebar→False,stats→ToString[Count],boundary
→ToString[NOEDGE],box→{})

type–>ToString[voronoi]=The Main variable that changes the information provided. Option:
type→ToString[voronoi] Uses the areas of the Voronoi Cells to calculate an expected hexagonal
spacing with the same intensity (shortname ToString[vor]). Option: type→ToString[coordination] Uses
the number of facets each individual Voronoi polygon has (shortname ToString[coord]). Option:
type→ToString[BondOrder] Uses the neighbours –as defined by the Delaunaly Triangulation– to calculate
the BondOrderParameter[]. Default symmetry is (symmetry–>6) but can be manually set to any variable.

symmetry –> 6 : Sets the symmetry number associated with the BondOrderParameter[]. No effect with any (type).

cells –> {} : This option provides a way to manually pass VoronoiCells[]
that have been precalculated. It is meant to save time by passing the automatic
VoronoiCells[] call for a large systems that might be run many times through this function.

points –> True : A graphics option that includes the centroids
of the particles on the final plot. These can be turned off with this option.

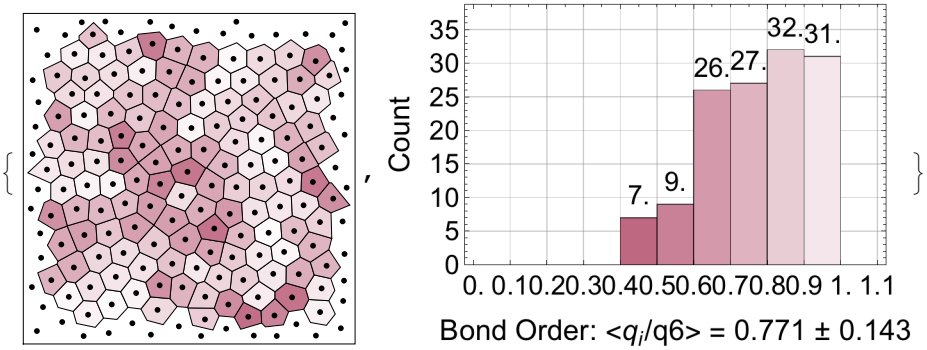
scalebar –> False : An option to include the scalebar assocciated with the colour code of (type).

stats –> ToString[Count] : Sets the type of stats passed into VoronoiHistogram[]. Recommended
settings – ToString[Count] or ToString[Probability]. See 'hspec' Option for Histogram[].

boundary –> ToString[NoEdge] : Settings for boundary corrections. Default boundary→ToString[NoEdge]
automatically removes any Voronoi Cells that lay on or outside of (box). Options include:
boundary→ToString[periodic] includes edge Voronoi polygons by adding periodically translated
neighbours outside of the box (shortname pbc). boundary→ToString[image] includes edge Voronoi
polygons by adding virtual particles that produce Voronoi cells with facets exactly on the edge of
(box). This effectively truncates or clips the edges of the Voronoi cells to the (box). (shortname img).

box –> {} : Explicitly defines the edges of a box. Note! – setting a
polygon will not change the (boundary), as it will default boundary→ToString[NoEdge]
which autodetects the box from the data. Remember to set a (boundary) option.

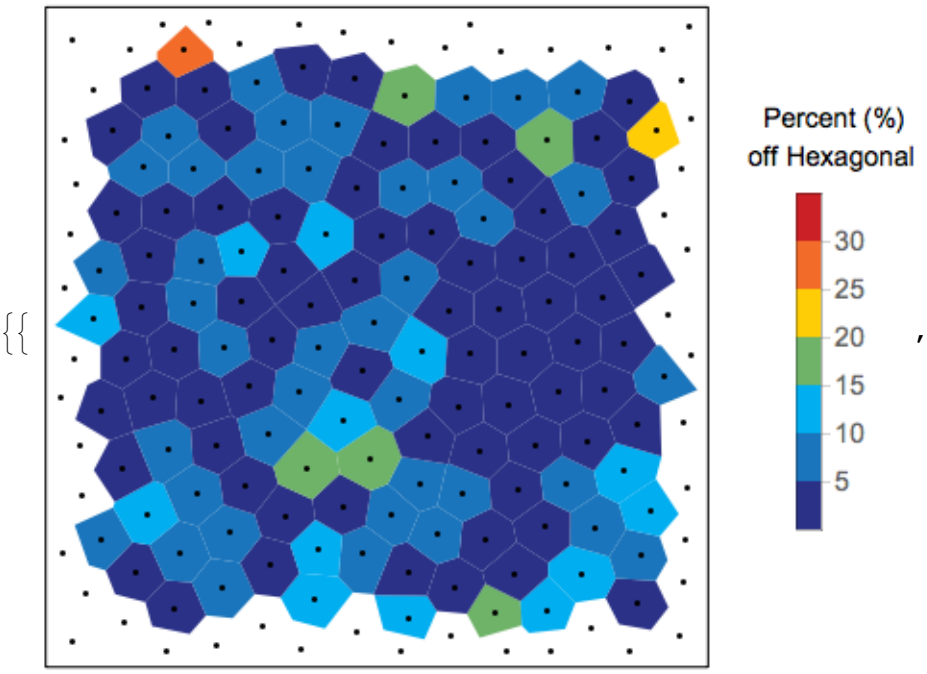
```
(*  Basic Plot for the Voronoi Tessellation                    *)
(*  Returns the Image of the Tiles and the Histogram of the data *)

PlotVoronoiTessellations@xylene2000
```

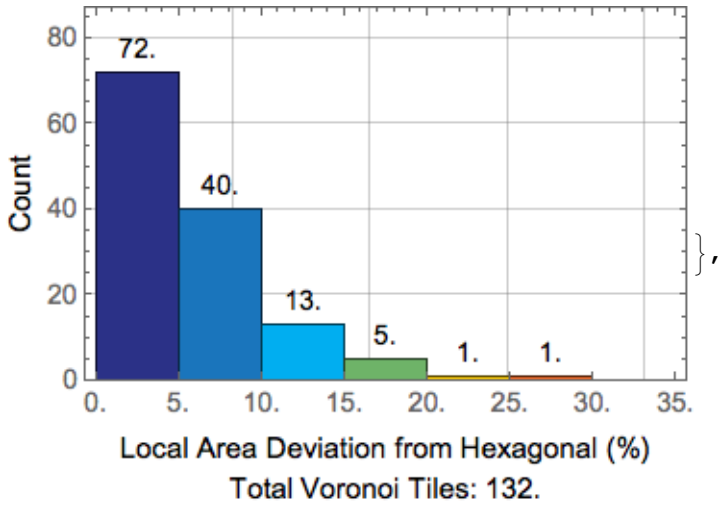


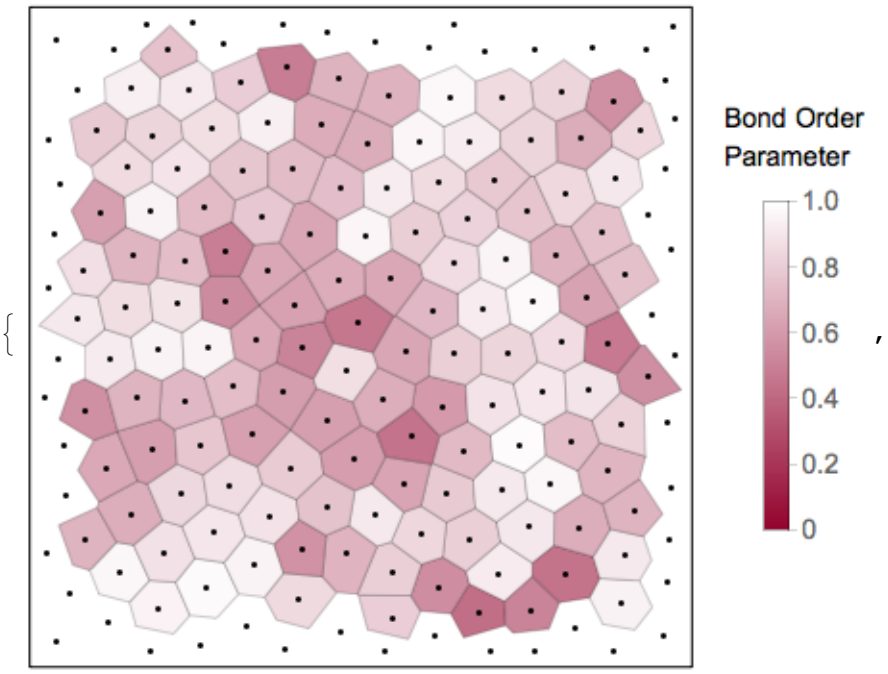
In[59]:=

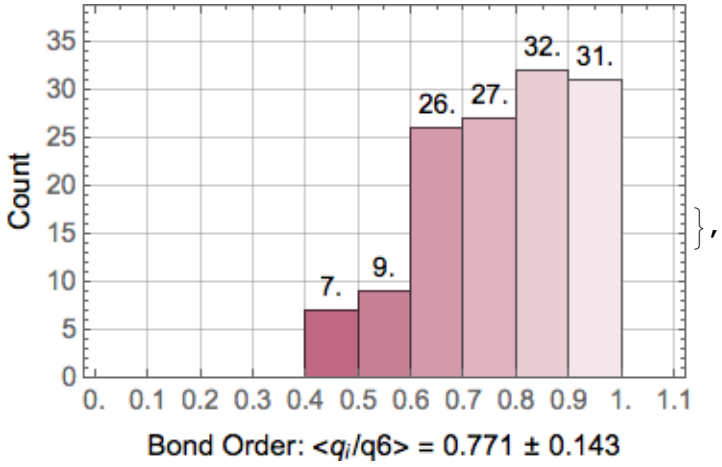
```
(* Additional Option #1 - type *)
(* Change the colour scheme of the Voronoi Tiles *)

PlotVoronoiTessellations[xylene2000, scalebar → True, raster → True, type → #] & /@
 {"vor", "bop", "coord"}
```

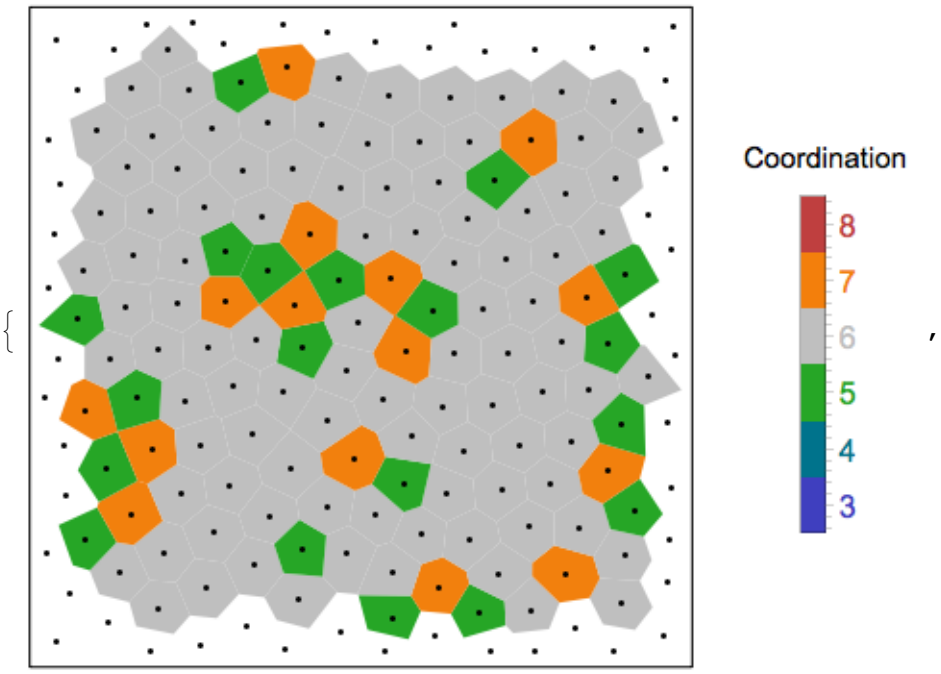
Out[59]=

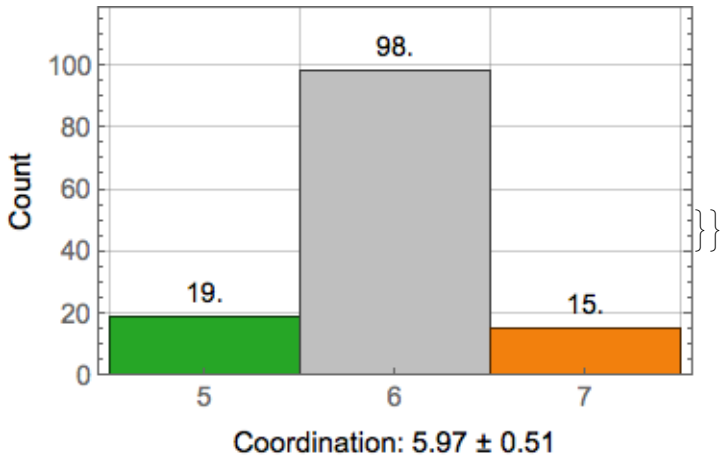



72.
40.
13.
5.
1.
1.
Count
0
20
40
60
80
0.
5.
10.
15.
20.
25.
30.
35.
Local Area Deviation from Hexagonal (%)
Total Voronoi Tiles: 132.

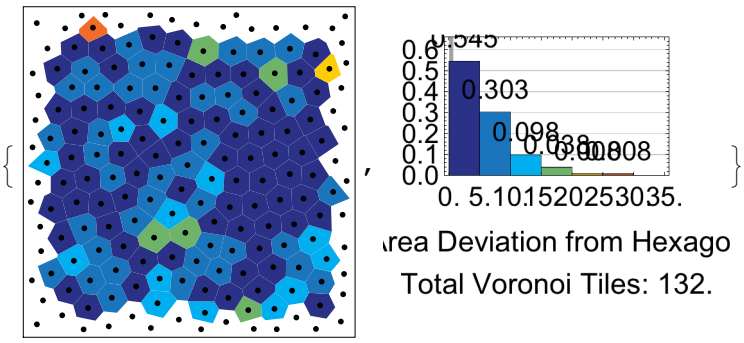

Bond Order
Parameter
1.0
0.8
0.6
0.4
0.2
0


Count
35
30
25
20
15
10
5
0
7.
9.
26.
27.
32.
31.
0. 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1. 1.1
Bond Order: <q_i/q6> = 0.771 ± 0.143

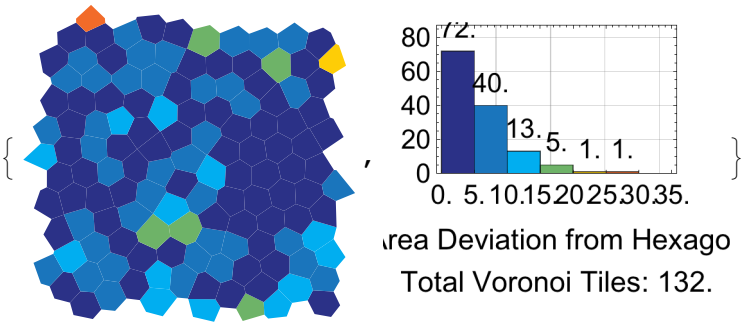

Coordination
8
7
6
5
4
3




```
(* Additional Option #2 - stats *)
(* Instead of Counting the Number of tiles, the Probability can be used. *)

PlotVoronoiTessellations[xylene2000, type → "vor", stats → "Probability"]
```



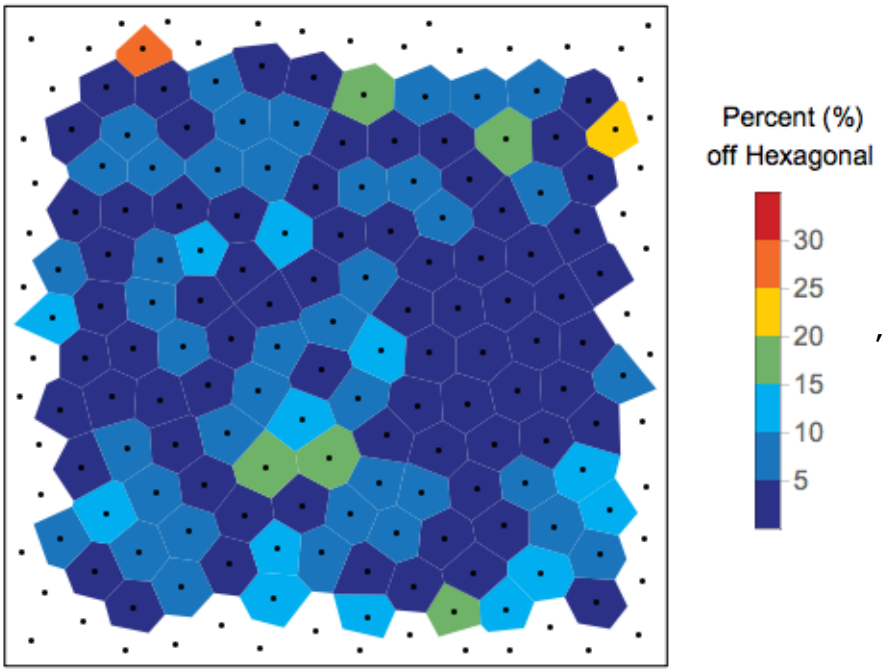

```
(* Additional Option #3 - points *)
(* Remove the points and lines to give it a more "stained glass" look *)

PlotVoronoiTessellations[xylene2000, type → "vor", points → False]
```

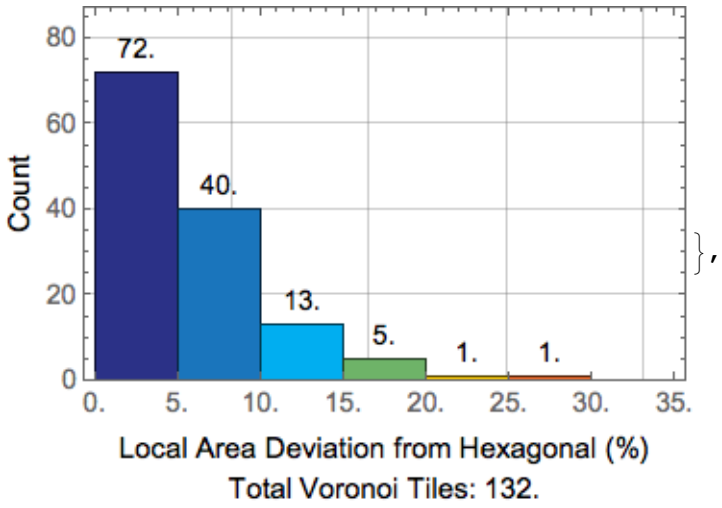


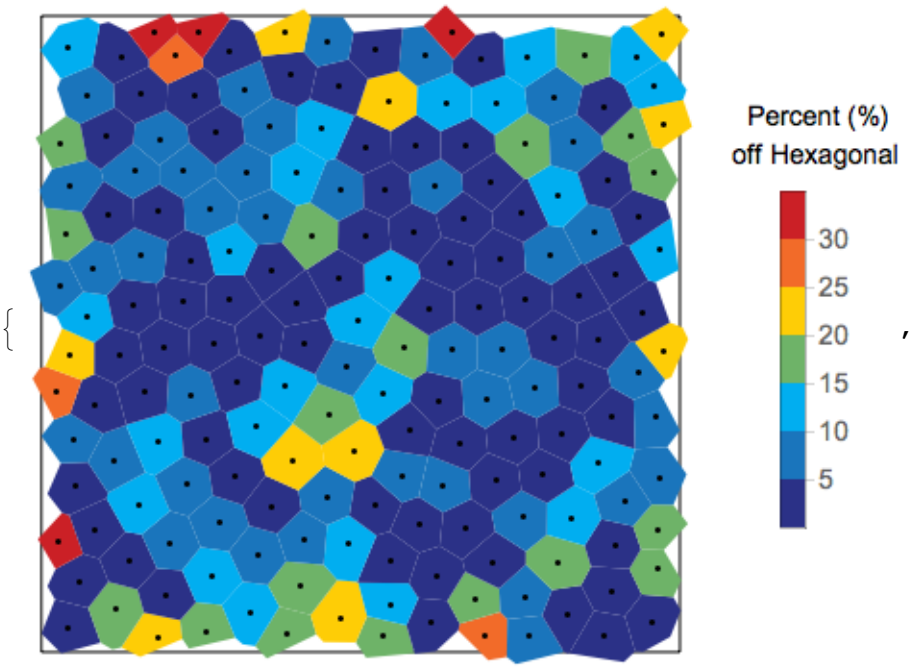
In[61]:=

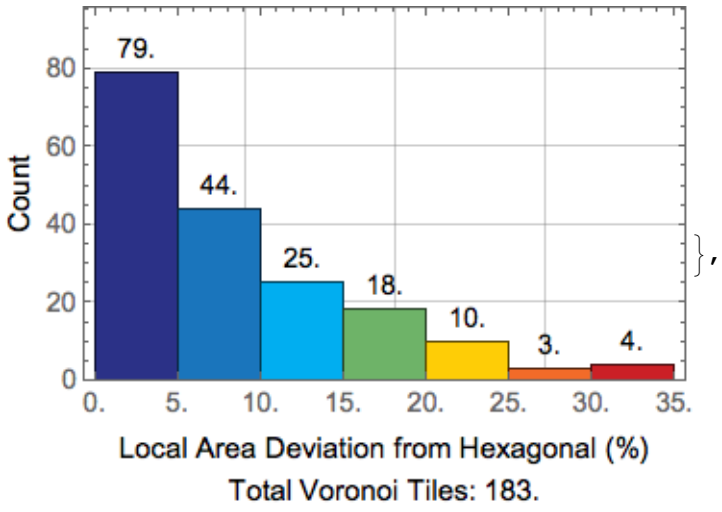
```
(* Additional Option #5 - boundary *)
(* Change the routine to sample points outside the edge *)
(* - noedge: removes any tiles that extend/touch the box *)
(* - pbc:  Applies Periodic boundaries to the edge,
total tile areas will total the box area *)
(* - image:  Places image charge particles
   outside so that the Voronoi tiles clip to the box *)

(* WARNING: type→"vor" depends on the global
  number density which changes with more particles *)

PlotVoronoiTessellations[xylene2000, type → "vor", scalebar → True,
   raster → True, boundary → #] & /@ {"noedge", "pbc", "image"}
```

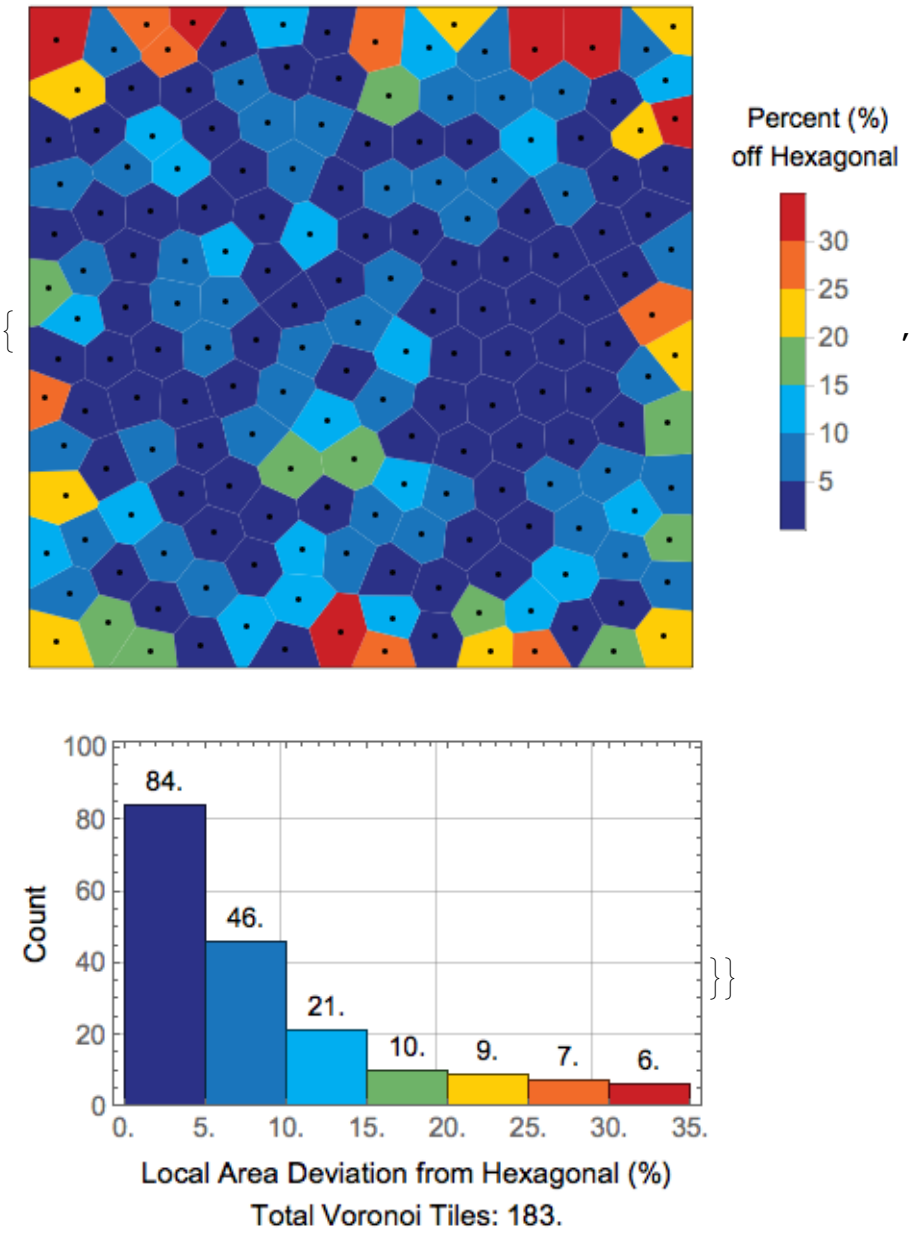
Out[61]=





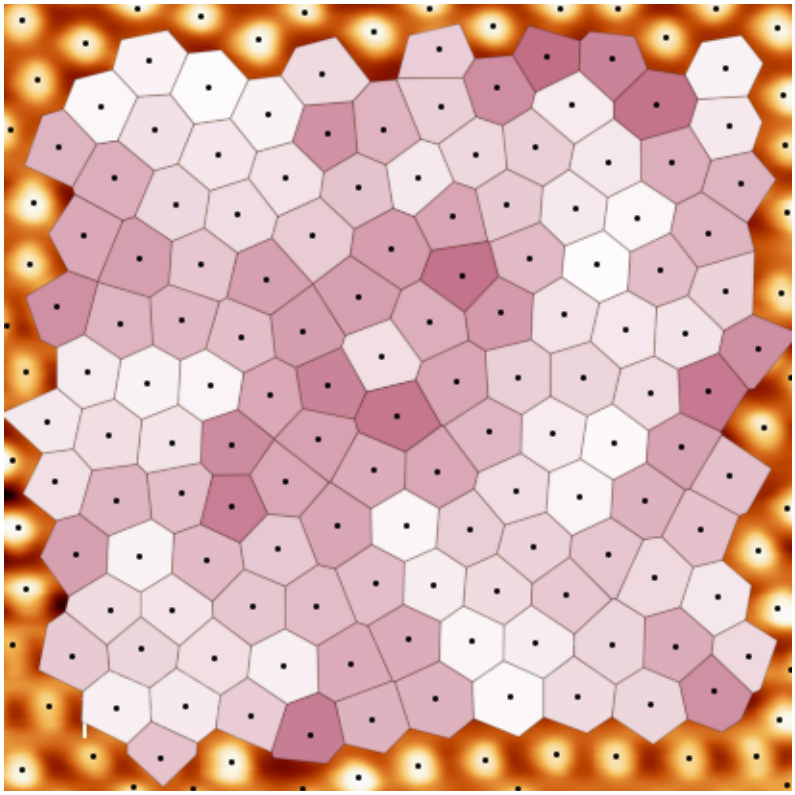

Percent (%)
off Hexagonal
30
25
20
15
10
5


79.
44.
25.
18.
10.
3.
4.
Count
0
20
40
60
80
0.
5.
10.
15.
20.
25.
30.
35.
Local Area Deviation from Hexagonal (%)
Total Voronoi Tiles: 183.

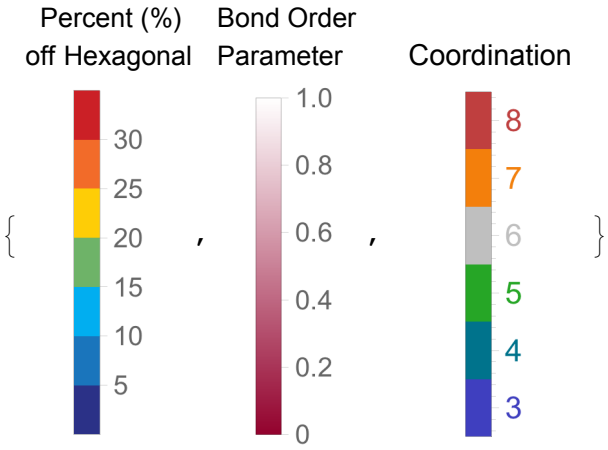



```
(*  Overlay the Nanoparticle Images with the Voronoi Tessellation:  *)
(* a) Image Dimensions tells how many pixels the image is  *)
ImageDimensions[images[[1]]]

(* b) Rescale the points by:  image/box  size  *)
vor = PlotVoronoiTessellations[(410 / 1000) * xylene2000][[1]];

(* c) The double ImageReflect is needed
  because the jpeg image {0,0} starts at the top left... *)
(*     ...while xy data starts in the bottom left as the origin.  *)
ImageReflect@Show[{ImageReflect[images[[1]]], vor }]
```

```
{410, 410}
```



```
(* Scale Bars can be called individually *)
ScaleBars[#] & /@ {"voronoi", "bop", "coord"}
```

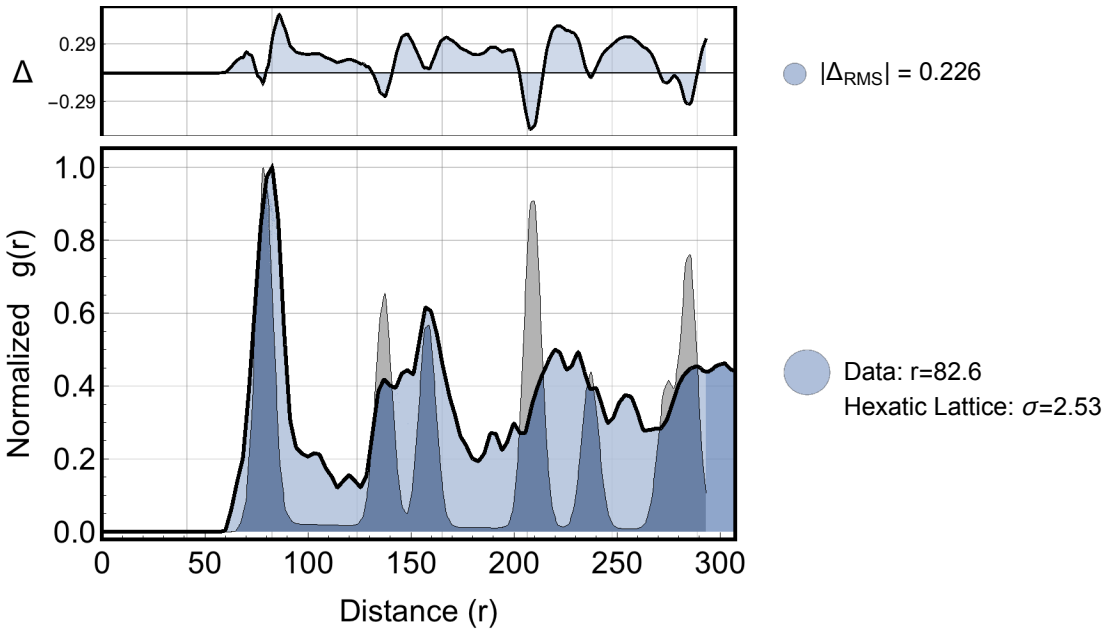


Pair Correlation Function - Distance between Particles

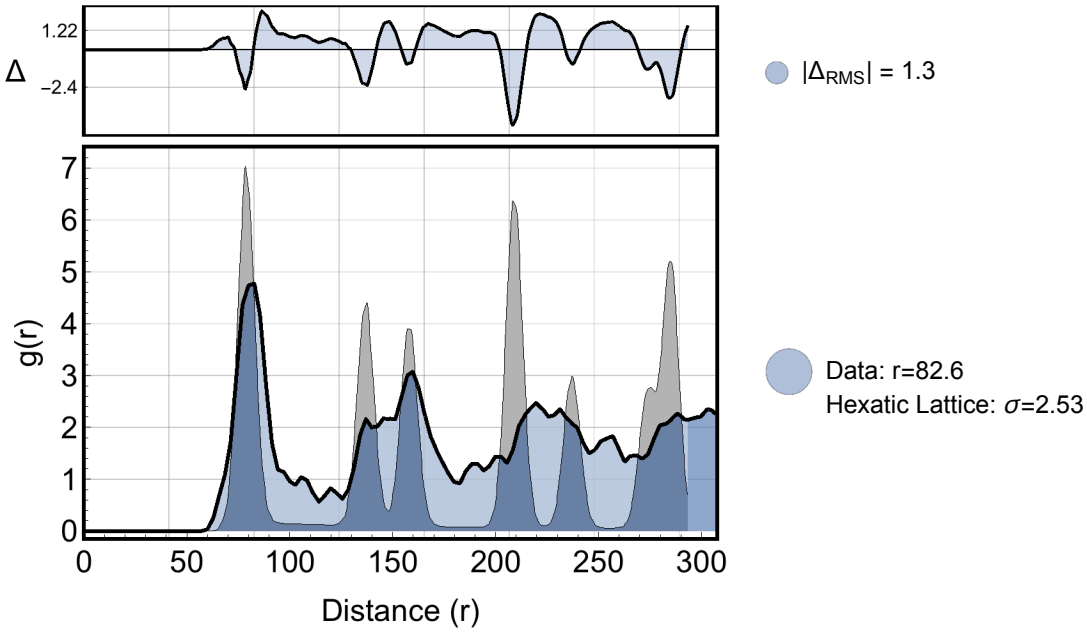
In[62]:= **? PairCorrelationFunction**

"PairCorrelationFunction[data2d , OptionsPattern[]]=Given a set of data2d={{x_1,y_1}...{x_n,y_n}},
returns a table {g(r),r} from r=0.0 to r=(maxBins * binSpacing). This is an ensemble
definition. Multiple data2d={{$conf_1$}...{$conf_n$}} with the same density can be input and will be
averaged.\n\nOptionsPattern=binSpacing→1,maxBins→1,box→{},edge→ToString[trunc],lattice→ToString[none],
hexNormalized→False.\nSelect edge corrections (edge→ #): ToString[pbc]
|| ToString[image] || ToString[noedge]\nChoosing lattice→ToString[hex] will Apply
the proper Periodic Boundaries when using HexagonalLattice[periodic → True]\n"

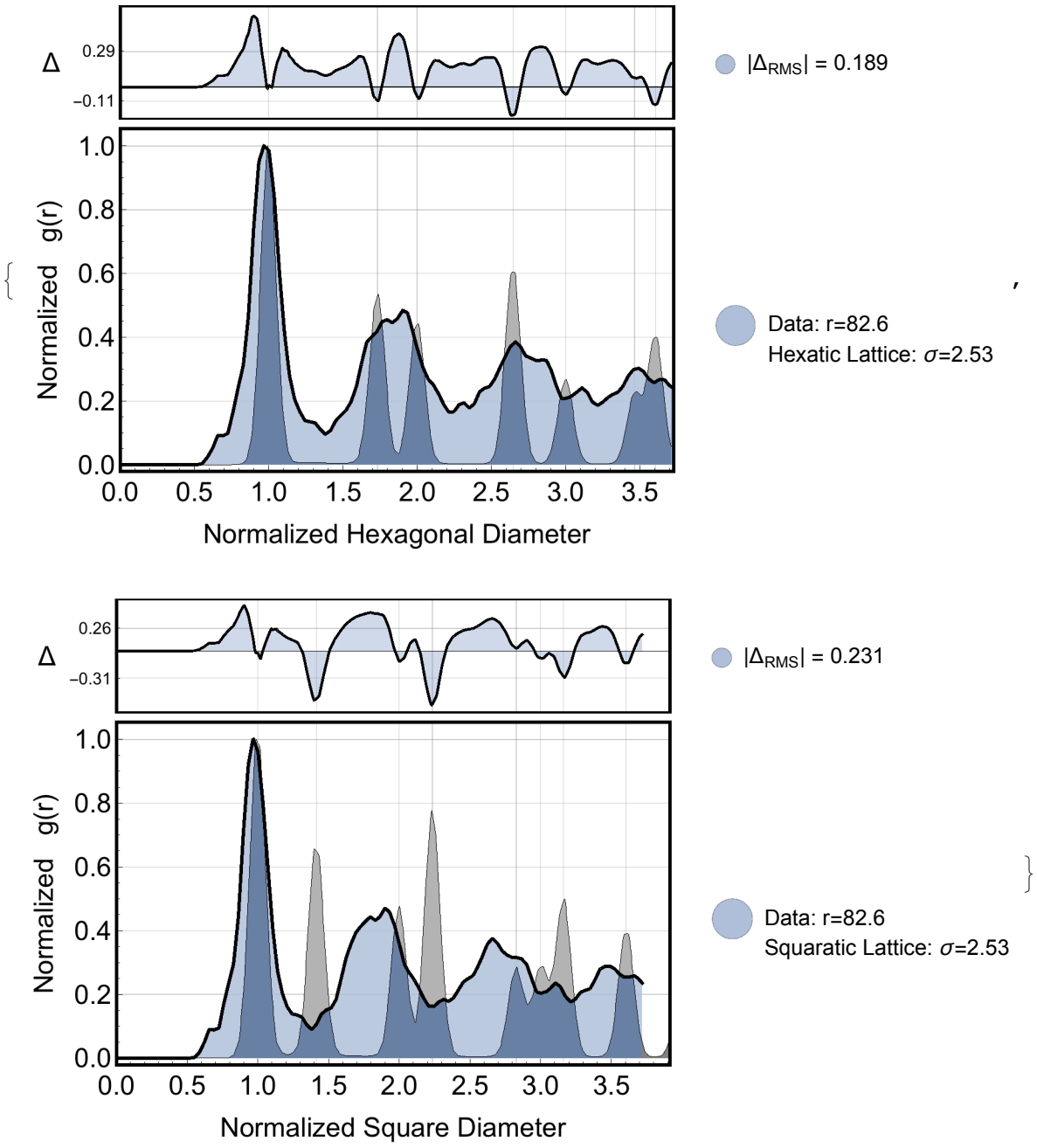
```
(*  Basic Plot for the Pair Correlation Function                    *)
(*  Returns the Plot of the first-
 peak normalized g(r) thats Smoothed + Hexatic Lattice *)
(* May take some time to complete:  (1-2 mins for large data sets) *)

PlotPairCorrelationFunction@xylene2000
```



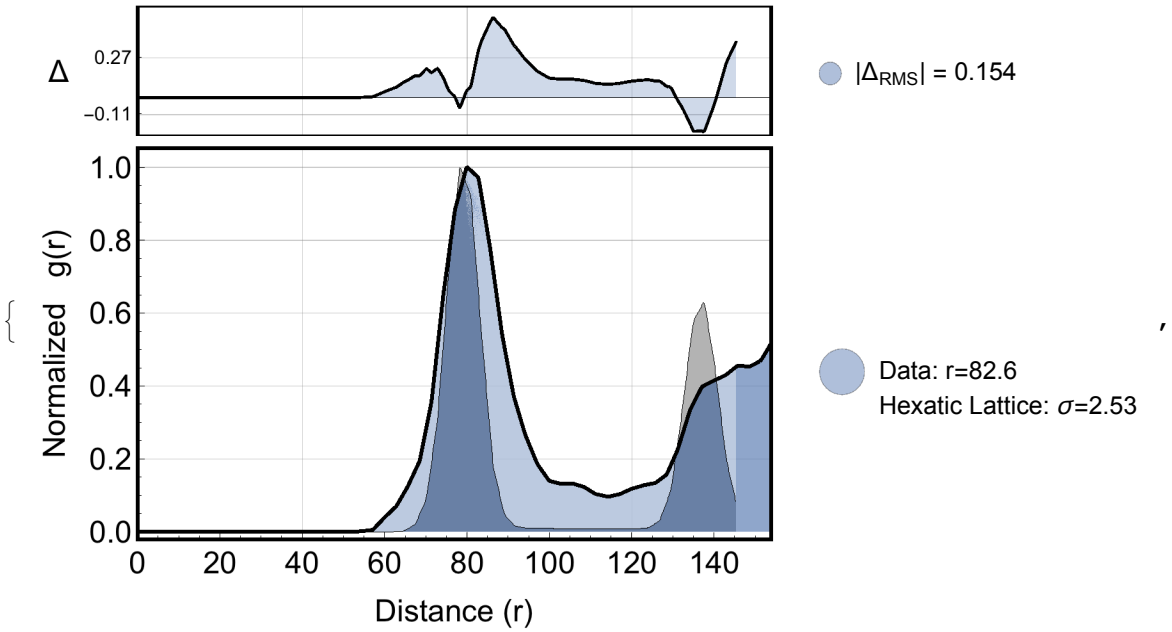
```
(* Additional Option #1 - normalized *)
(* Remove the normalization of the
 first peak to see the Absolute Value of g(r)  *)

PlotPairCorrelationFunction[xylene2000, normalized → False]
```

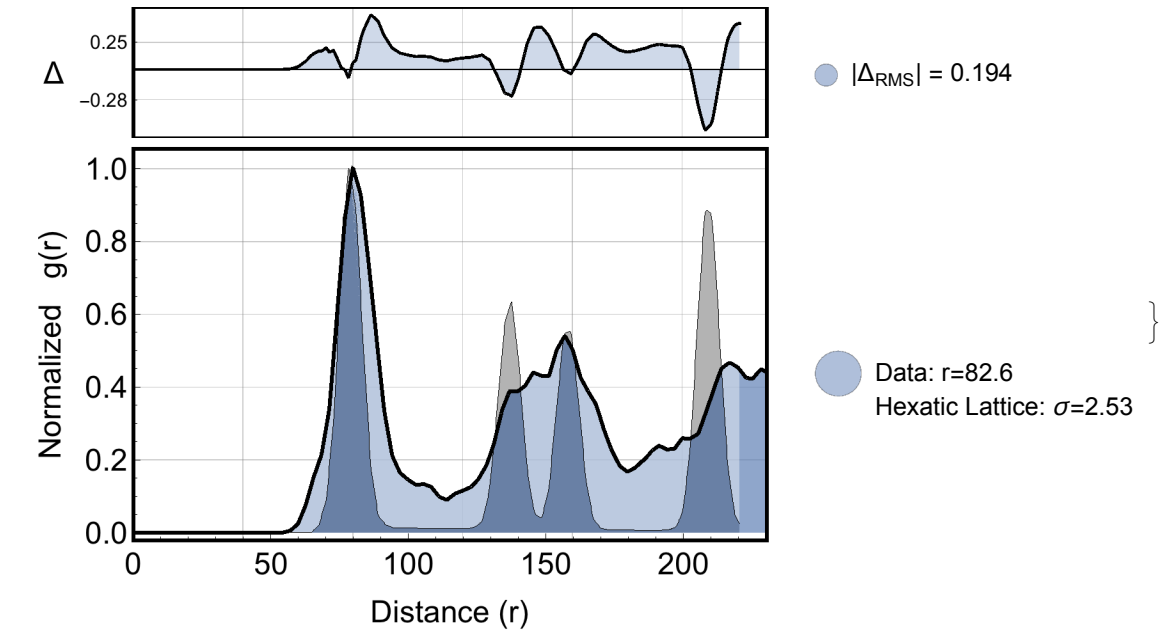


```
(*     Additional Option #2 - lattice                                  *)
(*     Normalizes the x-axis to the expected diameter                  *)
(*     Can choose the Reference Lattice:  "hex"  or "square"           *)
PlotPairCorrelationFunction[xylene2000, lattice → #] & /@ {"hex", "square"}
```

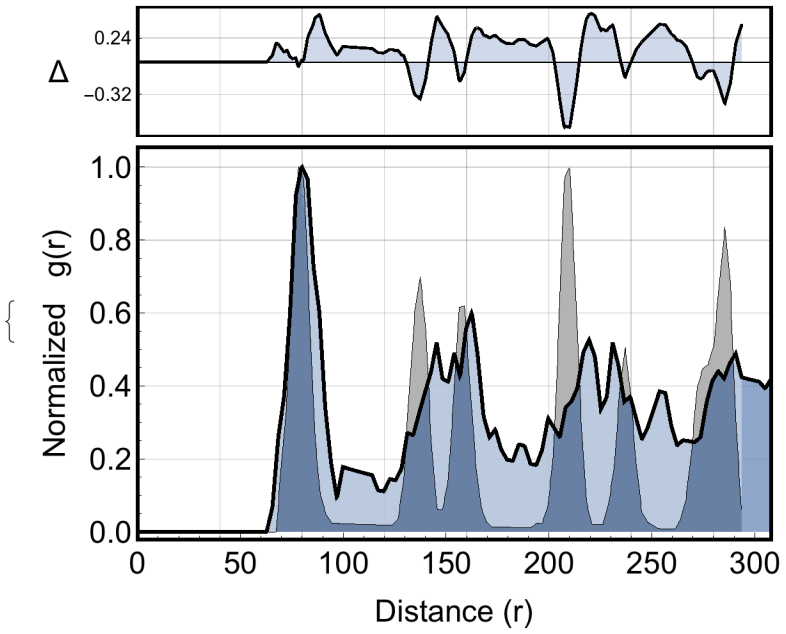


```
(*     Additional Option #3 - shells                                *)
(*     Vary the plotting distance with this parameter               *)
(*     Default Value = 4 shells                                     *)

(*    WARNING: If you ever get a divide by zero error (1/0)...      *)
(*     ... the first thing you should do is lower this value!!      *)
(*     Long range distances are bad for sparse data (N<200)         *)

PlotPairCorrelationFunction[xylene2000, shells → #] & /@ {2, 3}
```



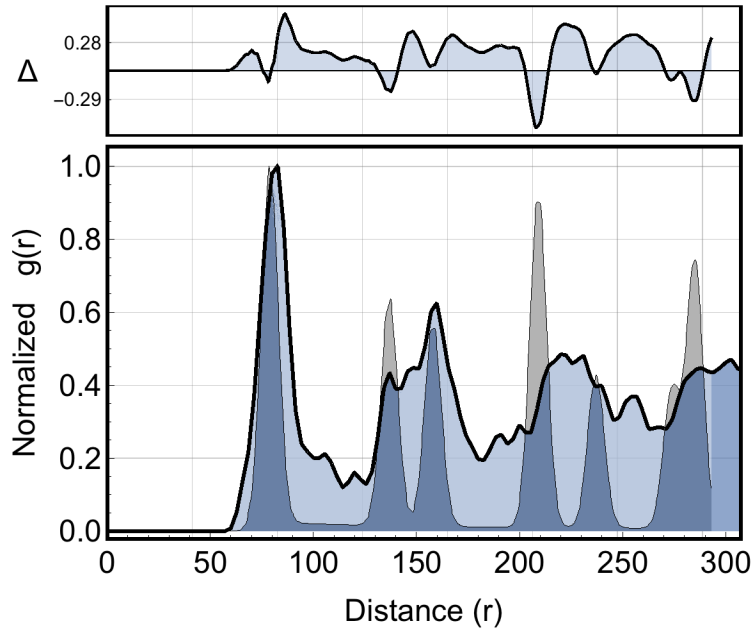


```
(*     Additional Option #4 - boots                                          *)
(*     Determines the Number of Randomized Displacements used to Smooth *)
(*     Default is 25                                                         *)
PlotPairCorrelationFunction[xylene2000, boots → #] & /@ {1, 200}
```



$|\Delta_{RMS}| = 0.22$

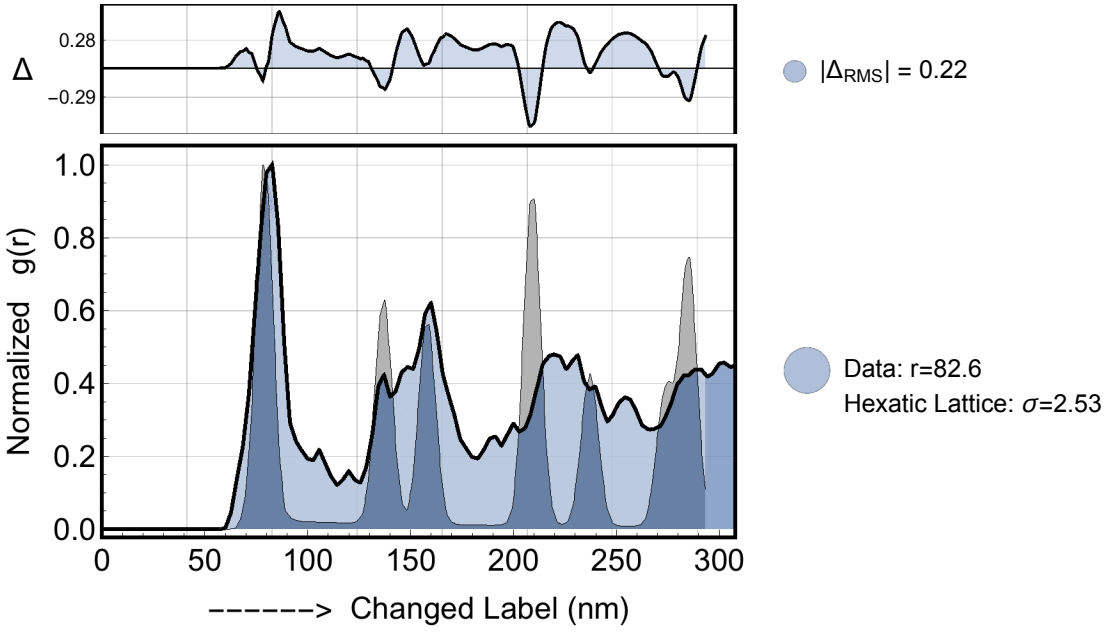
Data: r=82.6
Hexatic Lattice: σ=2.53



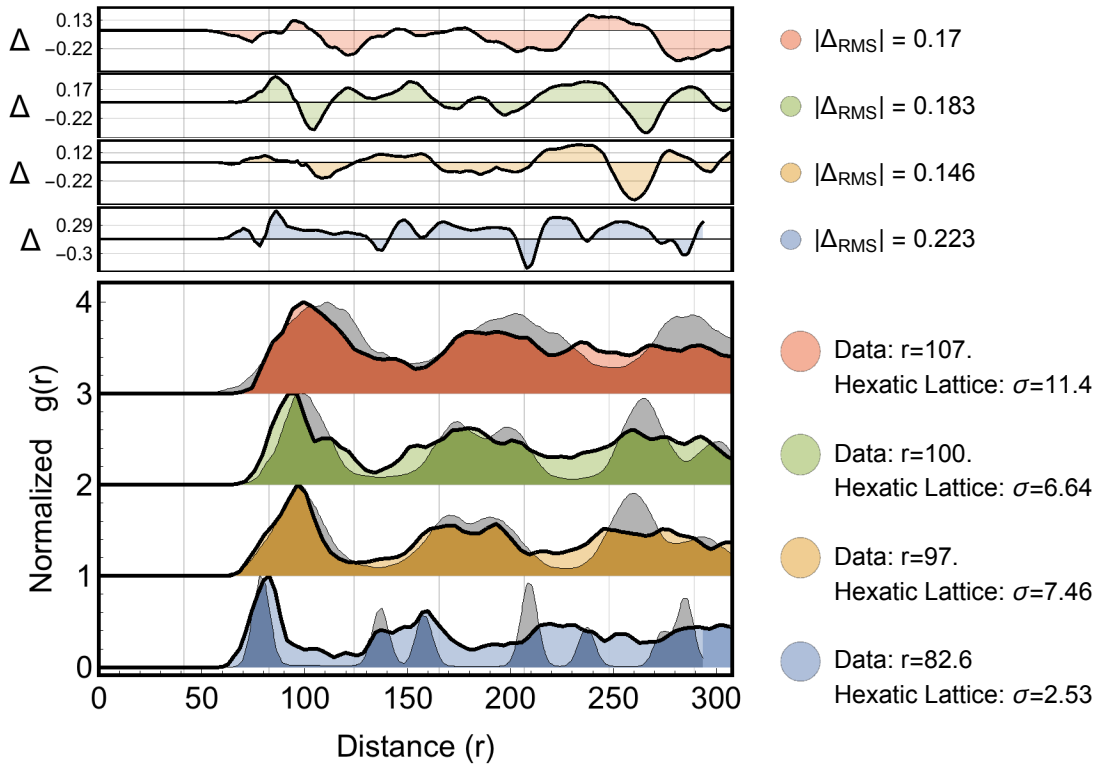
$|\Delta_{RMS}| = 0.224$

Data: r=82.6
Hexatic Lattice: σ=2.53

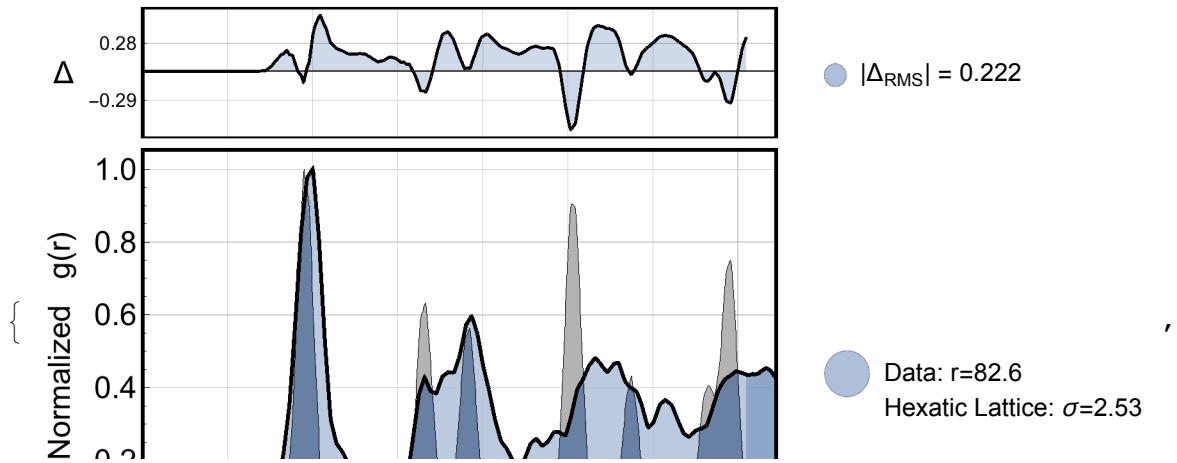
```
(*     Additional Option #5 - xLabel                    *)
(*     Change the x-axis label to have any string.      *)
PlotPairCorrelationFunction[xylene2000, xLabel → "------>  Changed Label (nm)"]
```

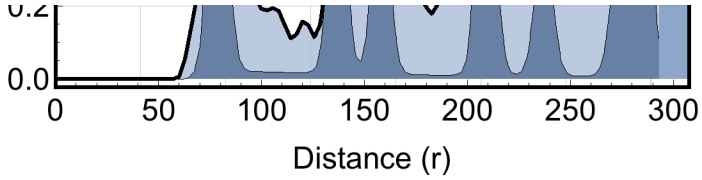


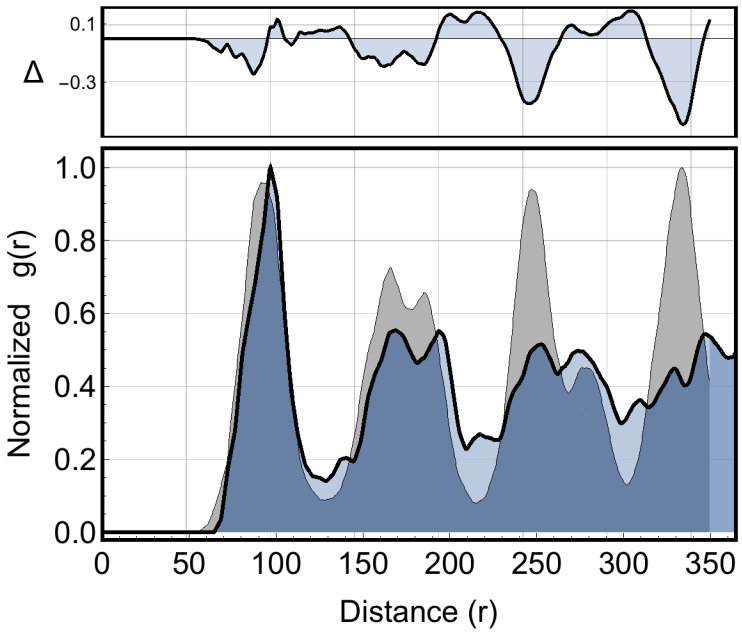
```
(*  Call in a List of Data:  *)
(* - Automatically detects multiple {x,y} data and plots it as a stack.  *)
(* - Residual functions at the top are Hexatic Lattice Substractions. *)
(* - All Options above work with this stacked version as well.  *)

PlotPairCorrelationFunction@xyXyleneList
```




```
(*     MAP in a List of Data:    *)
(* Returns the Individual Plots for each Configuration in the List *)

(*    Note the:  "/@"  NOT  "@"      *)

PlotPairCorrelationFunction /@ xyXyleneList
```

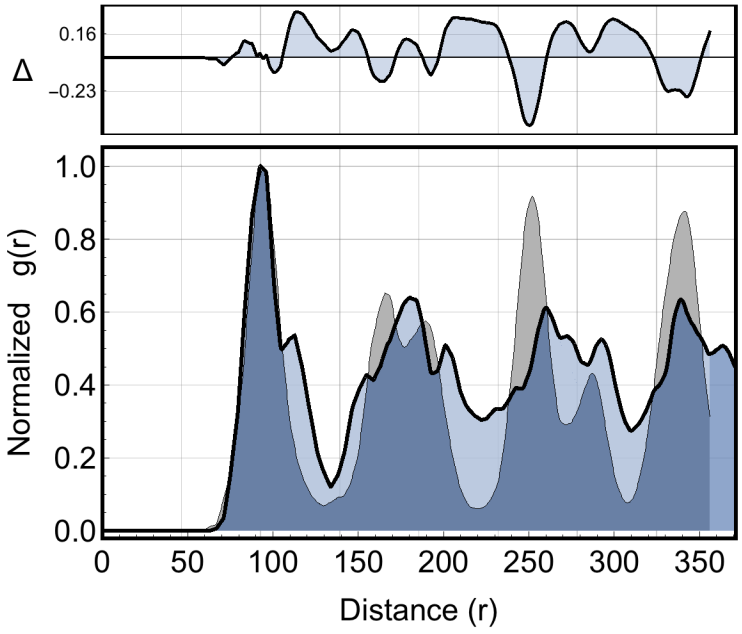






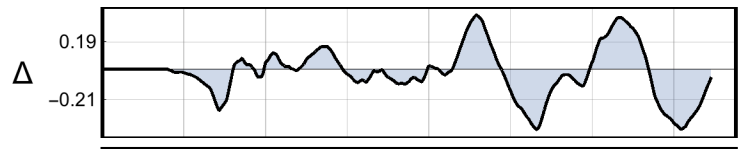
$|\Delta_{RMS}| = 0.173$

Data: r=97.
Hexatic Lattice: σ=7.46

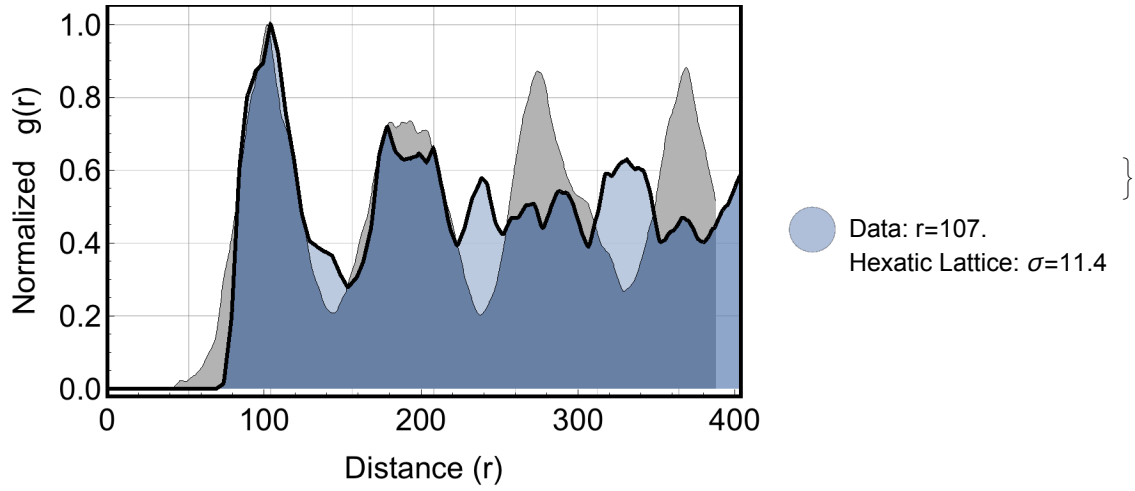


$|\Delta_{RMS}| = 0.164$

Data: r=100.
Hexatic Lattice: σ=6.64



$|\Delta_{RMS}| = 0.174$




```
(*    Distance Estimation from: Mathematica's Nearest[] Function   *)

AverageFirstNeighbourDistance /@ xyXyleneList
```

```
{71.3071, 82.635, 85.4448, 89.7071}
```

```
(*    Distance Estimation from: First Peak of g(r) - (no smoothing here)   *)

FirstPeakValue /@ (PairCorrelationFunction[#] & /@ xyXyleneList)
```

```
{82.8435, 96.5914, 96.1881, 103.78}
```

```
(*    Distance Estimation from: Voronoi Areas                              *)
(*    Returns:  { hexatic spacing,  lattice disorder parameter }   *)
ExpectedHexagonalDiameter /@ xyXyleneList
```

```
{{82.6236, 2.5267}, {97.0426, 7.45882}, {100.223, 6.63668}, {107.439, 11.4126}}
```

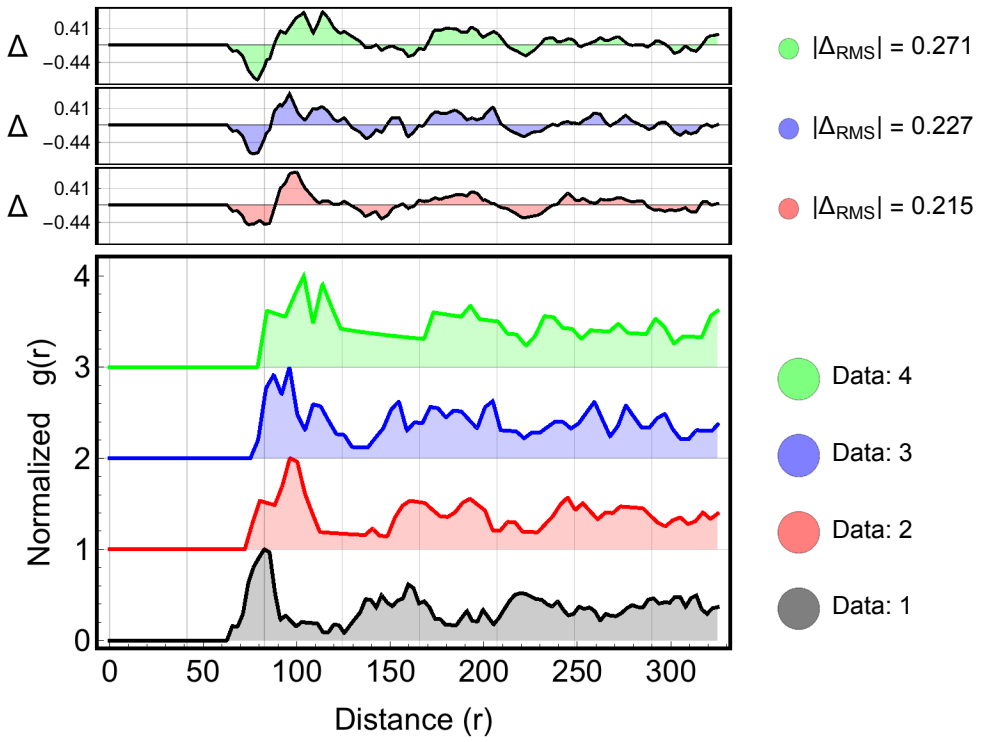
In[63]:=

```
? PlotPcfDifference
```

"PlotPcfDifference[PairCorrelationList , OptionsPattern[]]=Difference Spectrum of PairCorrelationFunction[]. The values for: ref={g(r),r} and func={g(r),r} need to be lists.\nOptionsPattern[]=(xmax→0,normalized→True,shapes→{},stacked→False,names→{},xLabel→{},refIndex→1)\n\n xmax → 1 : Cut−off distance for g(r) where r_{max}=xmax.\n\nnormalized → True : Automatic rescalling of the x−axis to\n\nshapes → {} : List of Polygons to be used as the Legend Markers where − shapes→{$polygon_1$, ... , $polygon_n$} \n\nstacked → False : Option to overlay curves, or to stack them with an offset. If stacked→True, it will produce the stacked version. Multiple PairCorrelationFunction[] can be set with: func={$g(r)_1$, ..., $g(r)_n$};\n\nxLabel → {} : String used to label the distance axis. If xLabel→ToString[Normalized Diameter], the function changes the gridlines to the expected positions of the hexagonal lattice.\n\nrefIndex → 1 : Defines which PairCorrelation[] in the list is chosen as the reference for all others to be subtracted from. "

In[64]:=
```
(*    Allows a comparison of any collection of graphs  *)
(*    Residual functions at the top
 are substractions relative to first data set.*)


PlotPcfDifference @ ( PairCorrelationFunction /@ xyXyleneList )
```

Out[64]=



Bond Order - Angular Orientation of Neighbours

In[65]:=
```
? BondOrderParameter
```

BondOrderParameter[unBoundedData2D , whichL , OptionsPattern[]]= Calculates the
Bond Order using Delaunay triangulation for neighbour definition. Defaults are to remove edge
particles and apply weighting of (voronoiBondFacet/totalVoronoiPerimeter) to every bond.

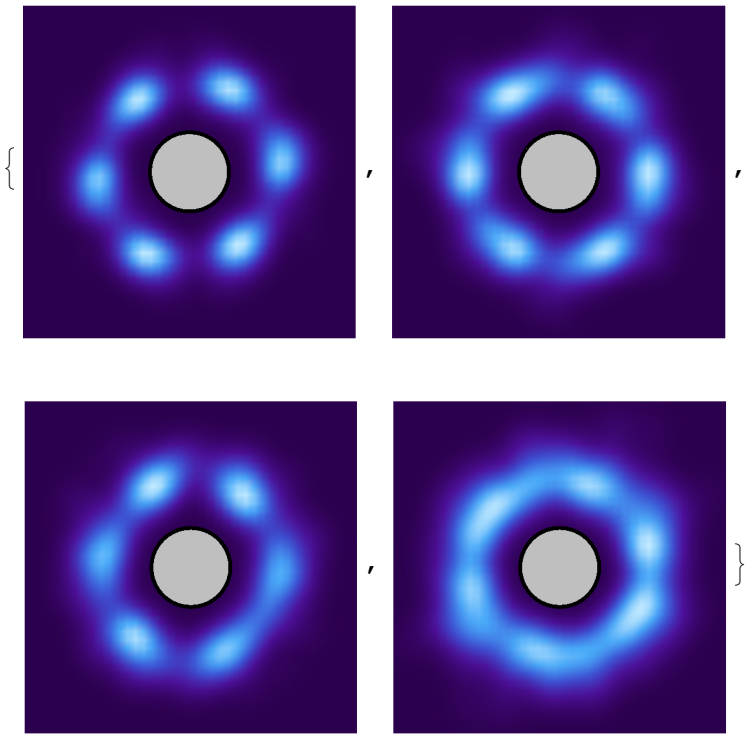
OptionsPattern=passVor→{},fast→True,edge–>ToString[NoEdge],vorbop→True,box→{},normalized→False,debug→False.

```
(*  Extract the local bond order parameter for each particle *)
(*  Call using: the data and symmetry number   *)

bop = BondOrderParameter[xylene2000, 6];
Mean[bop]
StandardDeviation[bop]
```

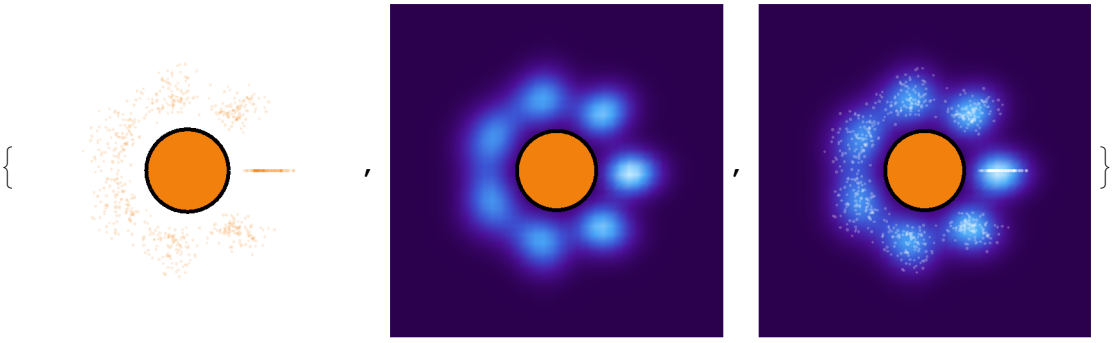
```
0.770507

0.142593
```

```
? CoordinationNeighbourCloud
```

```
(* Coordination cloud shows the probability
 of Neighbours relative to each object *)
(* Similar to the Fourier Transform,
except it can be separated by Coordination   *)

(CoordinationNeighbourCloud /@ xyXyleneList)[[All, 2]]
```



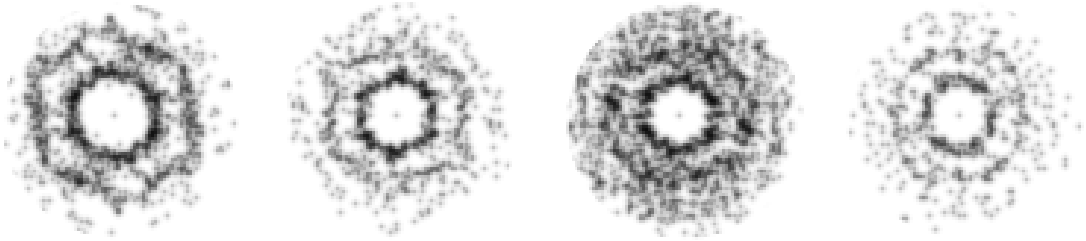
```
(*   Only select the particles that have 7 neighbours *)

CoordinationNeighbourCloud[xylene2000, coord → 7]
```



Diffraction - Correlation in Inverse Space

```
? DiffractionPatternFromPosition
```

```
(*  Plots the Diffraction (Fourier Transform) using a combination of:  *)
(*   ...Mathematica's ImagePeriodogram and ADO FFT (below)  *)

GraphicsRow[DiffractionPatternFromPosition /@ xyXyleneList, ImageSize → Large]
```



```
(*  Programmed FFT  *)

GraphicsRow[DiffractionPatternFromPosition[#, annulus → False] & /@ xyXyleneList,
 ImageSize → Large]
```