
ScatterSim Documentation

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The Nano Object is the base object for all ScatterSim code. It is comprised of known scattering.

It is defined in the following way:

```
from ScatterSim.NanoObjects import SphereNanoObject
sphere = SphereNanoObject(pargs=(dict(radius=2, rho_object=1.)))
```

where here `SphereNanoObject` is a `NanoObject` and `pargs` are the potential arguments of the nano object. In the case of a sphere, the only potential argument that describes it is its `radius` and `rho_object`, its density (this is normally electron density for xray scattering but can also be the `scattering length density`, as in neutron scattering).

1.1 Orientation and Placement

One of the powers of ScatterSim is the ability to place these NanoObjects in various positions and orientations, and compound them together. Before looking at how to compound objects together, we'll look at how we translate and rotate them.

1.1.1 Rotations

A `NanoObject` is first rotated. The rotations are defined through three `extrinsic rotations`, which is just a fancy way of saying that that the object is successively rotated about three different axes with respect to a **fixed** reference frame.

The rotations are as follows:

1. η : rotate the sample about the +z axis, counter clockwise in the x-y plane.
2. ϕ : rotate the sample about the +y axis, clockwise in the z plane.
3. θ : rotate the sample about the +z, counter-clockwise in the x-y plane

Each `NanoObject` will initially have some orientation with respect the the coordinate system, described in their docstrings. For example, the docstring of the `CylinderNanoObject` is defined as follows:

```
"""A cylinder nano-object. The canonical (unrotated) version
has the circular-base in the x-y plane, with the length along z.
"""
```

The rotations are defined by adding them to the pargs. For example, to rotate the cylinder such that it is aligned along the y-axis, and not the z-axis, one would do the following:

```
pargs = {
    'radius' : 3, # in nm
    'height' : 10, # in nm
    'eta' : 0, # 0 degrees about zaxis
    'phi' : 90, # 90 degrees about y axis
    'theta' : 90, # 90 degrees about z axis
}
cylinder = CylinderNanoObject(pargs=pargs)
```

This would re-orient the cylinder along the yaxis.

Note : The rotation is performed about the origin of the object's coordinate system. It is recommended that any new *NanoObjects* are defined so that their center of mass is aligned with the origin.

1.1.2 Translations

The translations are straight forward. They are always performed after the rotations of the objects and are defined by adding the x0, y0, and z0 parameters for x, y and z translations, respectively. For example, to now translate this cylinder along z by 10nm, one would add:

```
pargs = {
    'radius' : 3, # in nm
    'height' : 10, # in nm
    'eta' : 0, # 0 degrees about zaxis
    'phi' : 90, # 90 degrees about y axis
    'theta' : 90, # 90 degrees about z axis
    'z0' : 10, # translate +z by 10 nm
}
cylinder = CylinderNanoObject(pargs=pargs)
```

CHAPTER 2

Composite Nano Objects

CHAPTER 3

Lattice Objects

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- `modindex`
- `search`

4.1 Introduction

This documentation will help introduce how to use ScatterSim to model complex nano objects.