

BornAgain - Bug #1037

Doubling of unit cell in hexagonal lattice yields wrong results

13 Apr 2015 23:47 - a.glavic

Status: Archived	Start date: 13 Apr 2015
Priority: High	Due date:
Assignee: herck	% Done: 0%
Category:	Estimated time: 0.00 hour
Target version: Sprint 26	

Description

Simulations of a hexagonal cell of particles with only one particle in the unit cell generate a different output than the same particles placed 2x2 inside a unit cell of double lattice parameter.
As the physical sample is the same the resulting simulation should be the same, too.

As the file upload did not work properly I put example images and a script here:
<https://drive.google.com/folderview?id=0BzZkxCGgjeVsfmExbVM5U2I3WHVuTWFUNGf1aIFFcWxoSIM3RVladUNWWkxJMmxoYkV6LVU&usp=sharing>

History

#1 - 15 Apr 2015 16:44 - herck

- Status changed from New to Sprint

#2 - 15 Apr 2015 16:44 - herck

- Target version set to Sprint 26

#3 - 15 Apr 2015 17:19 - herck

- Assignee set to herck

#4 - 17 Apr 2015 15:06 - herck

- Status changed from Sprint to Resolved

#5 - 21 Apr 2015 17:01 - pospelov

- Status changed from Resolved to Archived

Files

HoneyComb_3_2x2_compare.py

5.17 KB

13 Apr 2015

a.glavic