

Miniproject Report

Summer Semester 2017

Self-Assembly of Core-Shell nanoparticles

This miniproject is in partial fulfilment (8 ECTS) of the M4 Module in the focal subject "Computational Material Science and Process Simulation"

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| Institute where miniproject was carried out | MSS |

Abstract

Core-shell nanoparticles have been extensively studied as potential candidates for a wide range of applications, including bioimaging, sensors, thermometry and more in recent years. Typically a core-shell nanoparticle has a multi-layered structure, consisting of a host core covered by one or several shells. Improvements in computer performance contributed to advances in the behavior of many body particle systems research. The simulation of core-shell nanoparticles has recently revealed interesting 2D structures that particles arrange in, which motivated this work to computationally study many body core-shell nanoparticle systems behavior in three dimensions.

The present work employs event-driven molecular dynamics to study core-shell particle self-assembly. Two simulation approaches are performed. In the first approach the shell potential is slowly being increased while shell-to-core ratio and packing density are kept constant. In the second approach a range of shell-potential vs packing density combinations is simulated at three different shell-to-core ratios. Two new particle crystal configurations are discovered. The first configuration represents modulated body-centered cubic structure. The second found configuration is an icosahedral quasi-crystal.

I hereby declare that this project report is my own work, that I have only made use of the cited and/or acknowledged documents/resources and that this report has not been previously submitted as academic coursework elsewhere.

Erlangen, 29.09.2017



Miniproject Report**Summer Semester 2017****Self-Assembly of Core-Shell nanoparticles****Grading Sheet**

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| Student's Name | Trunov, Mikhail |
| Matriculation Number | 22245933 |
| Grade awarded: | |
| Comments: | |

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| City, Date | Signature of supervising professor or lecturer with permission to examine |
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Note to grader: Please fill in and sign this form and return by mail or electronically to Dagmar Senft (MAP Office or dagmar.senft@fau.de) within 1 month after the submission.