Prof. Andre Schleife - Collaborative Design of Semiconductor Nanocrystals

This page captures information about our support of Prof. Andre Schleife's faculty fellowship.

Overview

Title: Computational Infrastructure for Collaborative Design of Semiconductor Nanocrystals

Link: http://www.ncsa.illinois.edu/about/fellows_awardees/computational_infrastructure_for_collaborative_design_of_semiconductor_nano

PI: Professor Andre Schleife, PhD (MatSE)

Co-PIs: Michal Ondrejcek, PhD (NCSA)

In short, the fellowship is exploring the development of the data science infrastructure that will enable a new computational/experimental approach to semiconductor nanocrystal (SNC) design.

Updates

4/23/2018

- Final Presentation by Andre

4/20/2018

- test data created without students knowing the details, run through the system and avaluate the most sensitive parameter
- script with MDF pipeline

4/06/2018

- ask Ben for the closed space on Petrel
- check GitHub repository and documentation
- ask NCSA for hosting the VM on Nebula

3/30/2018

- TBD

3/16/2018

- progress in web dashboard
- Neural network and Random forest outputs discussed
- MDF as an storage output, API, space etc.

3/9/2018

- Engineering Open House (EOH) presentations, viewing of molecules
- 3d goggles

3/2/2018 4pm

- getting ready for EOH, 3d goggles with molecules

2/16/2018 4pm

- Matlab (Igor) code for Gaussian curves

2/2/2018 4pm

- 'dummy' Gaussian fitting predictions using Neural Network
- front end discussed
- Engineering Open House app for visualizing molecules

12/13/2017 3:30pm

- Argonne visit with Andre Schleife (presentation)

12/8/2017 3:30pm

- Gaussian fitting predictions using Random Forest discussed
- front end
- GitHub repository

12/1/2017 3:00pm

- look at the metadata (JSON) of experimental curves

11/17/2017 3:00pm

- Friday meeting

11/10/2017 3:00pm

- Friday meeting

11/7/2017 3:00pm

- Attended Faculty Fellows reception at NCSA

10/11/2017 3:00pm

- introductory meeting with Andre Schleife in MatSE

References