Scientific Computing & Modelling

Quality Software. Quantum Science.

Seminar and workshop:

Materials modeling with the ADF modeling suite

Fedor Goumans, SCM
Friday August 15th, 9am-4pm
Room 1145, Engineering Building
Michigan State University, Hosted by Dr. Yue Qi

MICHIGAN STATE UNIVERSITY

Outline: The Amsterdam Density Functional (ADF) modeling suite is tailored for understanding and predicting structure and reactivity in chemistry and material science.

New features in the upcoming 2014 release and future plans will be discussed.
Bring your own laptop to get started with hands-on examples.

Program

9-10am: Overview of the features and benefits of the ADF modeling suite, with an emphasis on materials modeling.

The molecular (ADF) and periodic (BAND) DFT codes and the fast, approximate DFT module (DFTB) and reactive MD (ReaxFF) method will be introduced.

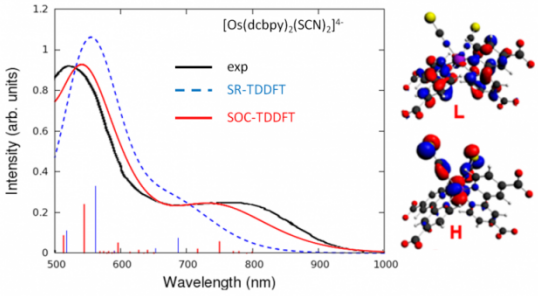
10-10.30am: Installing ADF modeling suite on laptops

10.30-12am: Introduction to periodic DFT with BAND
DFTB tutorial: lattice opt, phonons, DOS

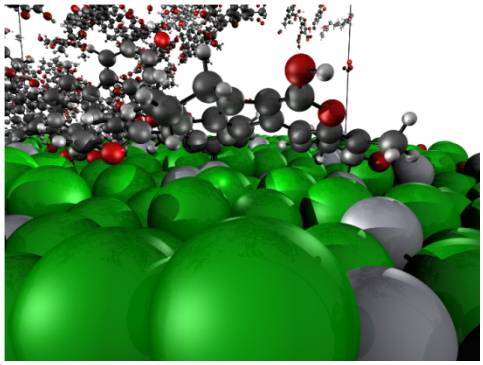
12-1pm: Lunch

1-4pm: Exercises or own examples according to interest, including ReaxFF tutorials and advanced teaching examples

Attendees will get a two-months demo license to further evaluate the ADF modeling suite.



Spin-Orbit Coupling increases DSSC efficiency



ReaxFF: MoNi-catalyzed coal combustion

Background:

ADF has a track record of almost 4 decades in providing excellent DFT software. With our team of highly trained chemists and physicists and active collaborations with academic development groups we continue to expand the functionality of our software. We offer expert scientific support.

Fedor (goumans@scm.com) has a broad background, ranging from photochemistry through inorganic chemistry (PhD 2005), astrochemistry, to quantum TST. He has been working for SCM since 2012.