Seminar
Chemistry & materials science with the ADF Modeling Suite

SCM
Software for Chemistry & Materials

Fri 26 August 2016, 11.30am, Room 115, Beckman Institute, Caltech
Dr. Fedor Goumans & Dr. Ole Carstensen, SCM
Hosted by Prof. William A. Goddard III

Outline: Fedor & Ole will discuss the capabilities of the ADF Modeling Suite, focusing on applications in chemistry, materials science and chemical engineering.

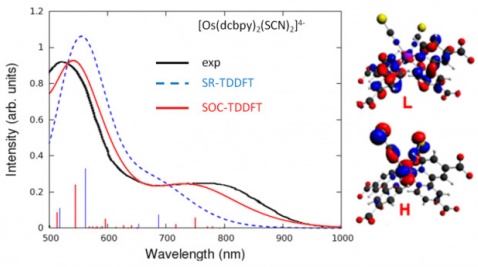
Key benefits of SCM's density functional theory programs for molecular (ADF) and periodic (BAND) systems are reviewed as well as density-functional based tight binding (DFTB), reactive MD ReaxFF and fluid thermodynamics with COSMO-RS.

Strong points and unique features will be highlighted with recent literature examples, in particular:

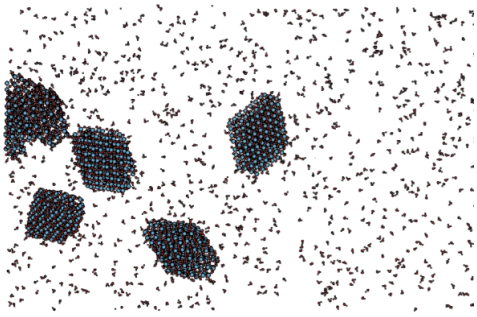
- Relativistic effects
- Spectroscopic properties
- Bonding analysis
- Proper 1D and 2D periodicity
- Trajectory analysis and ReaxFF parameterization

Furthermore, ongoing collaborations and EU projects will be shown, in particular with respect to scripting.

ADF is user-friendly software with a hassle-free single binary, synergy between the modules and an integrated graphical interface. After the seminar there is time for a GUI demo, as well as further discussions.



Spin-orbit coupling increases DSSC efficiency: J. Phys. Chem. C, 118, 17067



ReaxFF: TiO_2 nanoparticle aggregation
Nano Lett. 14, 1836-1842

Background:
Our team of highly trained chemists and physicists is passionate to make computational chemistry work for you. We offer expert scientific support and keep expanding capabilities through active collaborations with academic partners. The ADF Modeling Suite installs easily on Windows, Mac or Linux with an integrated GUI.

Both Fedor and Ole have a broad background in various areas of computational chemistry and as such love discussing scientific problems in chemistry & materials science. Fedor is business developer and Ole is support scientist at SCM.