

# Seminar

## Chemistry & materials science with the ADF Modeling Suite



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.

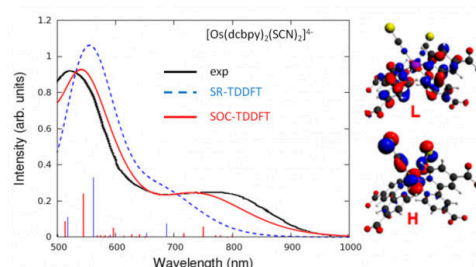
Key benefits of SCM's density functional theory programs for molecular ([ADF](#)) and periodic ([BAND](#)) systems are reviewed as well as density-functional based tight binding ([DFTB](#)), reactive MD [ReaxFF](#) and fluid thermodynamics with [COSMO-RS](#).

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

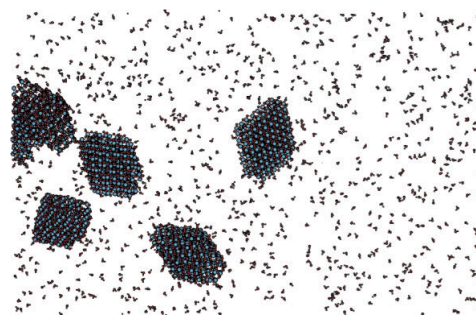
- Relativistic effects
- Spectroscopic properties
- Bonding analysis
- Proper 1D and 2D periodicity
- Trajectory analysis and ReaxFF parameterization

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<sub>2</sub> 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.