Hands-on Workshop
Chemistry & Materials Science with the ADF Modeling Suite

SCM
Software for Chemistry & Materials

Hosted by: Dr. Jan-Ole Joswig, TU-Dresden

Tutors: Mirko Franchini (franchini@scm.com)
Dr. Thomas Soini (soini@scm.com)

Monday, March 27, 2017, 10.00-17.00, HSZ/203

Outline: The ADF Modeling Suite is a powerful computational chemistry software for understanding and predicting structure and reactivity in chemistry and material science. The capabilities of the ADF modeling suite will be outlined, followed by hands-on examples.

Participants should register via email: theory@chemie.tu-dresden.de

Program

10.00-10.45: Introduction to the ADF Modeling Suite

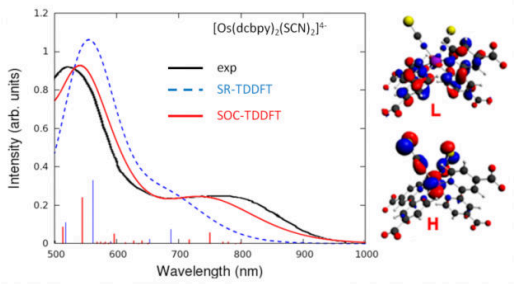
Overview SCM modules and graphical interface: molecular (ADF) and periodic (BAND) DFT, approximate DFT (DFTB), reactive MD (ReaxFF) and fluid thermodynamics (COSMO-RS).

10.45-11.00: Coffee break

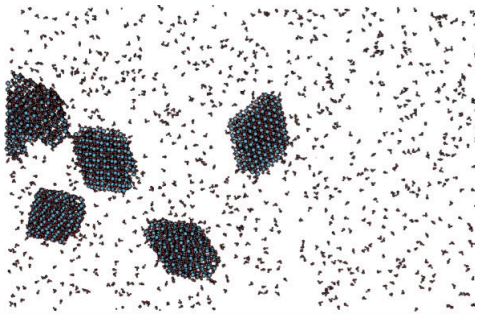
11.00-12.30: GUI introduction hands-on & demo

12.30-14.15: Lunch

14.15-17.00: Hands-on session covering advanced topics, opportunity for one-to-one discussion about specific research topics



SOC increases DSSC efficiency
J. Phys. Chem. C, 118, 17067



ReaxFF: TiO_2 nanoparticle aggregation
Nano Lett. 14, 1836

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.

Mirko's background covers theoretical solid state physics. At SCM he contributed many important technical improvements in ADF and BAND and is currently working on improving the user experience in the ADF modeling suite

Thomas obtained his PhD in theoretical chemistry on DFT methods with reduced self-interaction and their application to large metal clusters. He joined SCM in 2015 where he works on scripting environments and geometry optimization methods.