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

SCM Software for Chemistry & Materials

Hosted by SHARCNET, University of Waterloo

Tutor: Dr. Thomas Soini (soini@scm.com)

Monday, June 12, 2017

Outline: The ADF Modeling Suite consists of powerful computational chemistry software for understanding and predicting structure and reactivity in chemistry and material science. In this workshop the capabilities of the ADF modeling suite will be outlined, followed by hands-on examples covering basic features as well as a selection of more advanced examples.

Program

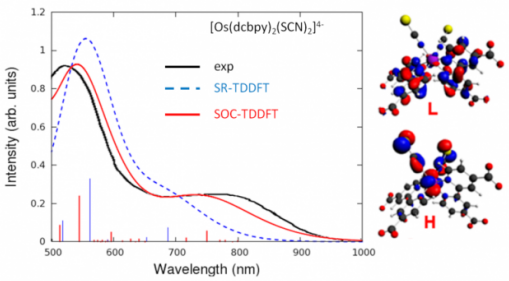
13.00-13.30: Introduction to the ADF Modeling Suite

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

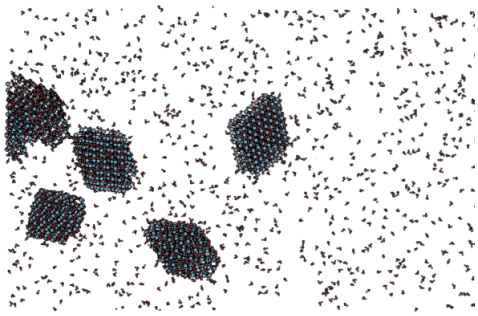
13.30-14.30: GUI introduction hands-on & demo

14.30-15.00: Break

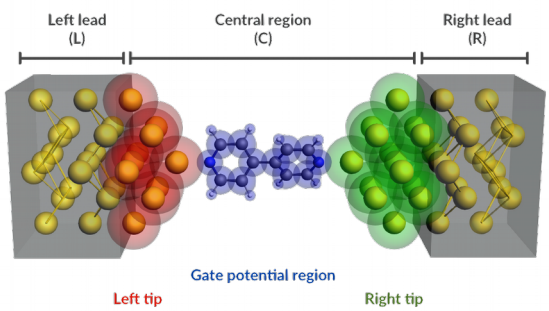
15.00-17.30: Hands-on session covering advanced topics (spectroscopy & relativistics, electron transport, reaction network analysis)



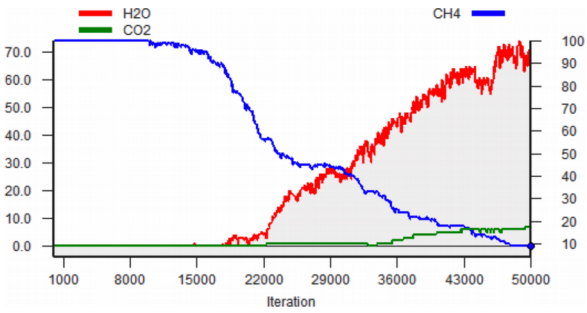
SOC increases DSSC efficiency
J. Phys. Chem. C, 118, 17067



ReaxFF: TiO_2 nanoparticle aggregation
Nano Lett. 14, 1836



Graphical NEGF model setup



ChemTrayZer species detection

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.

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 currently works on scripting environments and geometry optimization methods.