Seminar
Chemistry & materials science with the ADF Modeling Suite

SCM
Software for Chemistry & Materials

Mon 20 February 2017, 2-3pm,
Unilever Lecture Theatre, Chemistry Building
Cambridge University
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UNIVERSITY OF CAMBRIDGE

Outline: An overview of the ADF Modeling Suite, focusing on applications in chemistry & (nano)materials science. Time for demo & discussions afterwards.

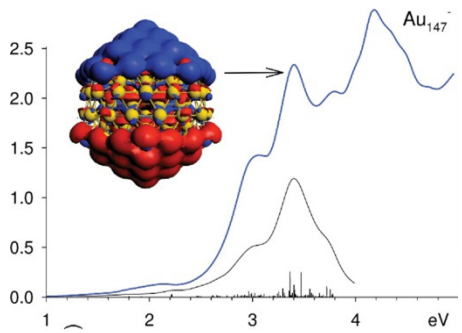
Key benefits of SCM's density functional theory programs for molecular (ADF) and periodic (BAND) systems are reviewed as well as density-functional based tight binding (DFTB), reactive MD ReaxFF and fluid thermodynamics with COSMO-RS.

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

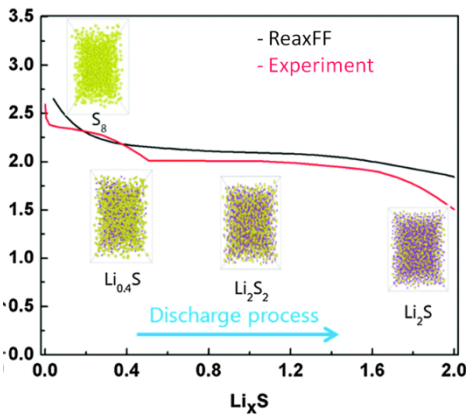
- Relativistic effects
- Spectroscopic properties: NMR, SERS, UV/VIS, XAS
- Bonding analysis
- Proper 1D and 2D periodicity
- Trajectory analysis and ReaxFF parameterization

Opportunities for collaborating, e.g. within EU projects will be discussed.

After the seminar there will be time to demo the user-friendly graphical interface to set up and analyze calculations for all modules. There is also plenty of time for further detailed discussions.



Plasmons in large nanoparticles with fast TDDFT : J. Phys. Chem. C, 120, 12773



ReaxFF: discharge in LiS battery
Phys. Chem. Chem. Phys. 17, 3383

Background:
The SCM 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.

Fedor has worked in various areas of computational chemistry and loves discussing how to tackle problems in chemistry & materials science. After his PhD in Amsterdam, post-docs in London and Leiden he started with SCM in 2012 as business developer.