Seminar: The ADF modeling suite 2014
Fedor Goumans, SCM
Friday August 8th, 2:00pm – 3:00pm
Room 401/402 Walter Library
Digital Technology Center,
University of Minnesota
Hosted by the Chemical Theory Center

Outline: The Amsterdam Density Functional (ADF) modeling suite is tailored for understanding and predicting structure and reactivity in chemistry and material science. New features in the upcoming 2014 release and future plans will be discussed.

Key features and benefits of SCM’s density functional theory programs for molecular (ADF) and periodic (BAND) systems are reviewed.

Strong points, in particular accuracy with relativistic effects, the wealth of calculable spectroscopic properties and chemical analysis tools will be highlighted.

Approximate, faster quantum-based methods for simulating large-scale complex systems will also be discussed:
• Density-functional based tight binding (DFTB)
• The reactive MD method ReaxFF
• Continuum method COSMO-RS for thermodynamic properties of fluids and solutions (solubilities, log P, pKa, ...)

There is ample time after the seminar to discuss matters further and/or to demonstrate setting up, running and visualizing calculations with the fully integrated GUI.

Background:
ADF has a track record of almost 4 decades in providing excellent DFT software. With our team of highly trained chemists and physicists and active collaborations with academic development groups we continue to broaden the scope and functionality of our software. We offer expert scientific support.

Fedor (goumans@scm.com) has a broad background, ranging from photochemistry through inorganic chemistry (PhD 2005), astrochemistry, to quantum TST. He has been working for SCM since 2012.