



**College on Multiscale Computational Modeling of  
Materials for Energy Applications  
4 - 15 July 2016**

***Co-sponsors: INRS Canada, ESF and Psi-k***

---

**First Principles Simulation of a  
Lithium-Air Interface for Battery Applications**

**Kurt STOKBRO**

QuantumWise A/S, Copenhagen, Denmark

Abstract:

Li-ion batteries are, at the moment, the most widely used in most most electric vehicles and hybrid electric vehicles. However, there are some disadvantages such as high price, slow charging, and low energy/power density. Li-air batteries are attracting attention due to the higher energy storing capacity and are being seen as possible alternative for Li-ion batteries. Nevertheless, still a lot of research has to be done in order to make Li-air battery competitive.

In this tutorial you will use the Virtual NanoLab (VNL) to build geometries and the Atomistix ToolKit (ATK) to simulate the properties of a Lithium-Air interface. You will learn how to cleave a surface and build an interface with VNL. The electronic structure will be calculated using the DFT-NEGF module in ATK.

The tutorial can be downloaded here:

[http://docs.quantumwise.com/tutorials/li\\_air\\_battery\\_interface.html](http://docs.quantumwise.com/tutorials/li_air_battery_interface.html)