



Contribution ID: 99

Type: **Workshop**

## **Materials Studio Mastery: A One-Day Dive into Advanced Modeling and Simulation**

*Monday, 4 December 2023 09:00 (1h 30m)*

This one-day tutorial on using Materials Studio is designed to provide participants with comprehensive hands-on experience in materials modeling and simulation. The tutorial will focus on several key aspects of Materials Studio, including setting up calculations in CASTEP and DMOL3, utilizing the adsorption locator, constructing surfaces, generating supercells and layers, and effectively interpreting simulation results.

The tutorial will begin with an introduction to the software environment and its capabilities. Participants will then delve into the intricacies of setting up calculations in CASTEP and DMOL3, two powerful tools for materials modeling. Subsequently, the tutorial will explore the adsorption locator feature, enabling participants to study the adsorption of molecules on surfaces.

A significant portion of the tutorial will be dedicated to building surfaces, understanding supercell generation, and constructing layers within the Materials Studio environment. Participants will gain practical skills in manipulating structures and simulating materials' behaviors under various conditions.

The tutorial will conclude with an emphasis on result interpretation, equipping participants with the ability to extract valuable insights from their simulations. Throughout the day, practical exercises and examples will be provided to enhance learning and ensure that participants leave with a strong foundation in using Materials Studio for materials research.

This tutorial is ideal for researchers, scientists, and students interested in computational materials science and seeking to harness the capabilities of Materials Studio for their work.

### **Student or Postdoc?**

Post-Doctoral

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**Session Classification:** Workshop 4

**Track Classification:** Computational Chemistry