We are pleased to announce a special 3-day training workshop that may interest students or other young researchers. The workshop is specifically targeted for students and other researchers who seek to learn fundamentals and practical usage of modern DFT based approaches, especially for application to research in interface science, catalysis and other materials for energy applications.

Lectures by users and invited guests will frame the subject, demonstrate examples of theory and experiment working together in research and introduce the theoretical methods.

Afternoons will be devoted to hands-on tutorials using the UVI cluster.

**DAY ONE**  
**Thursday September 10, 2015**

2:15pm to 4:15pm  
Session 1: *Computational Materials Science: Introduction to Linux*

4:15pm to 4:30pm  
Break

4:30pm to 6:30pm  
Session 2: *Vi the online editor*

**DAY TWO**  
**Friday September 11, 2015**

9:00am  
Session 3: *ASE interface*

11:00am to 11:15am  
Break

11:15am to 1:15pm  
Session 4: *GPAW and VASP*

1:15pm to 2:15pm  
Lunch
2:15pm to 4:15pm  Session 5: **Processing the simulations**
4:15pm to 6:15pm  Session 6: **Hands-on Session I: try your own system**

## DAY THREE
**Saturday September 12, 2015**

8:00 am to 9:00am  Session 8: **Introduction to High-Performance Computing**
9:00am to 9:15am  Break
9:15am to 11:15am  Session 10: **Hands-on Session II: analyze your own system**
11:15am to 11:30pm  **Review**
11:30 am to 12:30 pm  **Lunch**
12:30 pm to 1:15pm  Session 11: **Techniques Utilized for Creating NEXAFS spectrum-Data Reduction**
1:15pm to 3:00 pm  Session 12: **Hands-on Session III: Using IGOR pro, introduction to macros; Other software for NEXAFS –ATHENA etc**
3:00pm to 3:15pm  **Break**
3:15 pm to 5:00 pm  Session 13: **Hands-on Session IV: analyze your own synchrotron NEXAFS data**

## DAY FOUR
**Sunday September 13, 2015**

9:00am-10:45 am  Session 14: **NEXAFS theory and comparing and contrasting NEXAFS, XPS, EXAFS, IR and Raman.** New XAS techniques –Imaging NEXAFS, XMCD
11:00am to 11:15am  **Break**
11:15am to 12:00 pm  Session 15: **Hands on Session V and Review**