Contribution ID: **207** Type: **Workshop/BoF proposal**

High-throughput, atomistic multi-scale modeling with MedeA®-Universal Cluster Expansion (UNCLE) to study alloy structures, phase-stability and ordering

Sunday, 2 December 2018 11:00 (1h 30m)

Description:
MedeA-UNiversal CLuster Expansion (UNCLE) expands access to materials and properties at the meso and micro scales. Performing VASP ab-initio calculations on automatically chosen sets of small models, MedeA-UNCLE captures the configurational complexity of real materials at different temperatures by means of Monte Carlo random sampling. Tight integration with job control in MedeA guarantees stability and fault tolerance. Graphical tools monitor progress of fully automated simulations and allow a ready-for-use visualization of results.
Key Benefits of MedeA-UNCLE:
• Models systems containing millions of atoms with DFT accuracy
• User-friendly setup within MedeA Environment
• Workflow-based automation of cluster expansion refinement
• Efficient handling of hundreds of input structures
• Intuitive graphical analysis and visualization
• Split and restart complex calculations
• Extend and expand existing Cluster Expansions
Computational Characteristics:
• Use Genetic Algorithm or Compressive Sensing
• Full integration with MedeA-VASP and other modules
• High throughput using the JobServer
Properties from MedeA-UNCLE:
• Structures of stable phases
• Vacancy concentrations
• Miscibility
• Random mixing energy
• Phase stability as a function of temperature and concentration
• Solubility
• Order-disorder transition temperature
• Micro structure

Target Audience: This one day workshop is intended for undergraduate project students, postgraduate students, postdoctoral researchers and researchers who are familiar with the field and want to employ state-of-the art methodology based on the density functional theory to understand bulk materials properties, phase diagrams, order- disorder transition temperature, vancacy concentrations, miscibility and micro structure.

Type of tutorial: Mix of tutorials and hands-on (mostly practical)

Special requirements:
• Attendees need access to a laptop or workstation, active CHPC user account cluster.
• Open source spreadsheet such as Microsoft Excel with graphing capabilities is required for post-processing of output data.

Outline of full syllabus:
1. Introduction to the MedeA® Software environment

a. Structure retrieval, building
b. Flowchart interface
c. High Throughput support
2. Introduction to Cluster Expansion techniques
a. Theoretical background
b. MedeA® Uncle overview
3. MedeA® UNCLE hands-on (bulk)
a. Selected tutorials
4. MedeA® UNCLE hands-on (surfaces)
a. Selected tutorials
5. Q&A, wrap-up

Presenter Biography

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Session Classification: High-throughput, atomistic multi-scale modeling with MedeA®