

# Workshop on Computational Techniques in Materials Genomics

May 16 - 19, 2016

University of Florida - REEF

1350 North Poquito Road, Shalimar, FL 32579

## Program

### Monday, May 16, 2016 - Auditorium

- 8:30 - 8:45      **Opening Remarks**
- 8:45 - 10:15    **Part I - Introduction to Density Functional Theory - Basic algorithms and functionalities**, Dr. Marco Buongiorno Nardelli, University of North Texas
- 10:15 - 10:45    **Coffee Break**
- 10:45 - 12:15    **Part II - Introduction to Density Functional Theory - Basic algorithms and functionalities**, Dr. Marco Buongiorno Nardelli, University of North Texas
- 12:15 - 1:30     **Lunch Break**

### Afternoon Tutorial Sessions 1:30 - 5:00 - Room 117

- 1:30 - 3:00      **Tutorial**, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3
- 3:00 - 3:30      **Coffee Break**
- 3:30 - 5:00      **Tutorial**, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3

### Tuesday, May 17, 2016 - Auditorium

- 08:45 - 10:15    **Part I - Electronic and transport properties from atomic basis representations**, Dr. Marco Buongiorno Nardelli, University of North Texas
- 10:15 - 10:45    **Coffee Break**
- 10:45 - 12:15    **Part II - Electronic and transport properties from atomic basis representations**, Dr. Marco Buongiorno Nardelli, University of North Texas
- 12:15 - 1:30     **Lunch Break**

### Afternoon Tutorial Sessions 1:30 - 5:00 - Room 117

- 1:30 - 3:00      **Tutorial**, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3
- 3:00 - 3:30      **Coffee Break**
- 3:30 - 5:00      **Tutorial**, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3

### **Wednesday, May 18, 2016 - Room 117**

- 8:45 - 10:15** Part I - Lattice dynamics, dielectric properties and vibrational spectroscopies - novel functionals, Dr. Marco Fornari,
- 10:15 - 10:45** Coffee Break
- 10:45 - 12:15** Part II - Lattice dynamics, dielectric properties and vibrational spectroscopies - novel functionals, Dr. Marco Fornari
- 12:15 - 1:30** Lunch Break

### **Afternoon Tutorial Sessions 1:30 - 5:00 - Room 117**

- 1:30 - 3:00** Tutorial, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3
- 3:00 - 3:30** Coffee Break
- 3:30 - 5:00** Tutorial, Dr. Arrigo Calzolari, Istituto Nanoscienze CNR-NANO-S3

### **Thursday, May 19, 2016 - Auditorium**

- 8:45 - 10:15** Part I - High-throughput computational materials tools and databases, Dr. Marco Fornari, Central Michigan University
- 10:15 - 10:45** Coffee Break
- 10:45 - 12:15** Part II - High-throughput computational materials tools and databases, Dr. Marco Fornari, Central Michigan University
- 12:15 - 1:30** Lunch Break

### **Post-Workshop Seminars: Thursday, May 19, 2016, 1:30 - 4:30 - Auditorium**

- 1:30 - 2:15** DREAM.3D/SIMPL as a data management and analytics tool, Dr. Michael Groeber, Materials and Manufacturing Directorate, AFRL
- 2:15 - 3:00** Automated, data-driven characterization systems for autonomous materials quantification, Dr. Michael Groeber and Dr. Michael Uchic, Materials and Manufacturing Directorate, AFRL
- 3:00 - 3:30** Coffee Break
- 3:30 - 4:15** New analytics approaches to understanding metallic additive manufacturing for tailored design, Dr. Michael Groeber and Dr. Edwin Schwalbach, Materials and Manufacturing Directorate, AFRL
- 4:15 - 5:00** Networks of materials: Models and algorithms, Dr. Sergiy Butenko, Industrial and Systems Engineering Department, Texas A&M University