

# Workshop on Computational Techniques in Materials Genomics

May 16 - 19, 2016

University of Florida - REEF  
1350 North Poquito Road, Shalimar, FL 32579

This is a four-day workshop on “Computational Techniques in Materials Genomics”, which is organized by Intelligent Robotics, Inc (a non-profit research lab based in Tallahassee, Florida), University of Florida, and University of Central Florida for the Air Force Research Laboratory.

The workshop will facilitate and encourage collaboration between academic and government researchers with interest in the development of computational techniques based on the physics-based material models, innovative discovery of new materials with reduced development time, highly optimized performances, and more effective ways of transitioning the technology into production.

The agenda is comprised of a series of lectures in the mornings followed by practical tutorials in the afternoons. The lectures and tutorials will be conducted by **Dr. Marco Buongiorno Nardelli** (University of North Texas), **Dr. Marco Fornari** (Central Michigan University) and **Dr. Arrigo Calzolari** (Istituto Nanoscienze CNR-NANO-S3).

## Topics for the workshop include:

- *Introduction to computational materials science and materials genomics*
- *Introduction to density functional theory and quantum ESPRESSO*
- *Basic algorithms and functionalities*
- *Electronic properties and general post-processing algorithms*
- *Lattice dynamics*
- *Optical and dielectric properties, Raman and IR scattering*
- *Electronic and thermal transport*
- *High-throughput techniques in computational materials science and materials discovery*
- *The MTF (Medium throughput framework) and AFLOWLIB.org*

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

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

**PROGRAM:** The program will be updated on the workshop website:

<https://www.compgeom.com/workshop.html>

**REGISTRATION:** All interested researchers are welcome to attend the workshop; however, registration is required. There is no registration fee. The registration form is available on the workshop website:

<https://www.compgeom.com/workshop.html>

**IMPORTANT:** The participants are expected to bring their own laptops and be able to install Quantum ESPRESSO software.