

**Summer School Program  
Simulation of Complex Microstructure in Materials**

**May 19-24, 2013  
Gainesville, FL**

**Sunday, May 19**

6:00 – 8:00 pm Registration and Welcome (125 Rhines Hall)

**Monday, May 20**

8:00 – 8:30 Registration, 125 Rhines Hall

8:30 – 8:45 Welcome and Logistics (**Susan Sinnott, Simon Phillpot**)

8:45 – 9:30 Lecturer 1 (**Donald Brenner, NCSU** – Atomistic Simulations of Material Interfaces)

9:30 – 9:45 Break

9:45 – 10:30 Lecturer 1 (Part 2)

10:30 – 10:45 Break

10:45 – 11:30 Lecturer 2 (**Roger de Souza, Aachen** – Computational Studies of Complex Oxides for Energy Applications)

11:30 - 11:45 Break

11:45 – 12:30 Lecturer 2 (Part 2)

12:30 – 2:00 Lunch

2:00 – 2:30 Professional Development – Charge for developing research initiative (**Simon Phillpot, Florida**)

2:30 – 3:45 Student led working group (with faculty)  
1/3 discussion lectures – developing questions  
2/3 discussion of research of students

3:45 – 4:00 Break

4:00 – 4:40 Questions for Lecturers (1 and 2)

5:00 – 6:00 Meeting of the CAMS Advisory Board

## Tuesday, May 21

- 8:45 – 9:30 Lecturer 3 (**Krishna Rajan, Iowa State** – Microstructure and Materials Informatics)
- 9:30 – 9:45 Break
- 9:45 – 10:30 Lecturer 3 (Part 2)
- 10:30 – 10:45 Break
- 10:45 – 11:30 Lecturer 4 (**Izabela Szlufarska, Wisconsin** – Material Microstructure and Mechanics of Materials)
- 11:30 - 11:45 Break
- 11:45 – 12:30 Lecturer 4 (Part 2)
- 12:30 – 2:00 Lunch
- 2:00 – 2:30 Professional Development – How to develop field and transition into a new field (**Krishna Rajan, Iowa State**)?
- 2:30 – 3:45 Student led working group (with faculty)  
1/3 discussion lectures – developing questions  
2/3 discussion of student research initiative
- 3:45 – 4:00 Break
- 4:00 – 4:45 Questions for Lecturers (3 and 4)

## Wednesday, May 22

8:45 – 9:30 Lecturer 5 (**Steve Plimpton, Sandia** – Practical Aspects to Atomistic Simulations of Interfaces)

9:30 – 9:45 Break

9:45 – 10:30 Lecturer 5 (Part 2)

10:30 – 10:45 Break

10:45 – 11:30 Lecturer 6 (**Blas Uberuaga, LANL** – Modeling Grain Boundary-Defect Interactions in Ceramics)

11:30 - 11:45 Break

11:45 – 12:30 Lecturer 6 (Part 2)

12:30 – 2:00 Lunch

2:00 – 2:30 Professional Development – Ethics and Plagiarism/Working in Groups/Entrepreneurship (**Erik Sander or Bill McElroy – Leadership Institute, Florida**)

2:30 – 3:45 Student led working group (with faculty)  
1/3 discussion lectures – developing questions  
2/3 discussion of student research initiative

3:45 – 4:00 Break

4:00 – 4:45 Questions for Lecturers (5 and 6)

## Thursday, May 23

- 8:45 – 9:30 Lecturer 7 (**Mo Li, Georgia Tech**, Modeling Amorphous Solids)
- 9:30 – 9:45 Break
- 9:45 – 10:30 Lecturer 7 (Part 2)
- 10:30 – 10:45 Break
- 10:45 – 11:30 Lecturer 8 (**Anter El-Azab, Purdue** – Phase Field Modeling of Complex Microstructure)
- 11:30 - 11:45 Break
- 11:45 – 12:30 Lecturer 8 (Part 2)
- 12:30 – 2:00 Lunch and **Posters of Student Research (all School Participants)**  
Judges - **Roger deSouza, Steve Plimpton, Mo Li, Krishan Rajan**
- 2:00 – 2:30 Professional Development – What is life like as a professor (**Izabela Szlufarska**) and a national laboratory staff member (**Blas Uberuaga**)?
- 2:30 – 3:30 Student led working group (with faculty)  
1/3 discussion lectures – developing questions  
2/3 discussion of student research initiative
- 3:30 – 3:45 Questions for Lecturers (7-8)
- 3:45 – 6:00 Final preparations for student presentations (including dinner)
- 6:00 – Student Research Initiatives presented to Panel of Experts  
@ 20 minutes → 8:15
- Awards for posters and initiatives  
Reception

## Friday, May 24

8:15 – 9:00 Lecturer 9 (Muralikrishna Raju , Penn State - Applications of Molecular Dynamics, Metadynamics and Monte Carlo simulations using ReaxFF Reactive Force Fields to Aqueous Interfaces)

9:00 – 9:15 Break

9:15 – 10:00 Lecturer 10 (Susan Sinnott, Florida – Atomic Simulations of Heterogeneous Interfaces)

10:00 – 10:15 Break

10.15 – 11:00 Lecturer 10 (Part 2)

11:00 – 11:30 Student led working group (with faculty)  
Discussion lectures – develop questions

11:30- 12:15 Questions for Lecturers (9 and 10)

12:15-1:30 Lunch and Adjourn