

Program

June 3, 2019

- 08:00 -- 09:00 Arrival at Hardy Hall and Registration
09:00 -- 09:15 Opening Remarks (Chris Winstead, Dean, College of Arts and Sciences)

Introduction to Disordered materials

- 09:15 -- 10:05 **Tutorial 1:** Disordered materials: An introduction
Parthapratim Biswas (University of Southern Mississippi)
10:05 -- 10:55 **Tutorial 2:** Structural optimization of disordered materials
Raymond Atta-Fynn (University of Texas at Arlington)
10:55 -- 11:10 Break
11:10 -- 12:00 **Tutorial 3:** An Introduction to Linux for scientific computing
Sung Lee (The University of Southern Mississippi)
12:00 -- 13:00 Lunch
13:00 -- 15:00 Computer Lab Session I: Linux computing
Sung Lee (The University of Southern Mississippi)
15:00 -- 15:15 Break
15:15 -- 17:30 Computer Lab Session II: Structural optimization
Raymond Atta-Fynn (University of Texas at Arlington)

June 4, 2019

Monte Carlo and molecular dynamics simulations

- 8:30 -- 09:20 **Tutorial 4:** Structural and electronic properties of disordered solids
David Drabold (Ohio University)
9:20 -- 10:10 **Tutorial 5:** Introduction to Monte Carlo methods
Parthapratim Biswas (University of Southern Mississippi)
10:10 -- 10:20 Break
10:20 -- 11:10 **Tutorial 6:** Inverse and hybrid approaches to disordered solids
David Drabold (Ohio University)
11:10 -- 12:00 **Tutorial 7:** Introduction to molecular dynamics simulation
Raymond Atta-Fynn (University of Texas at Arlington)
12:00 -- 13:00 Lunch
13:00 -- 15:00 Computer Lab Session III: Inverse and hybrid modeling techniques
David Drabold + Dil Limbu (OU + USM)
15:00 -- 15:15 Break

15:15 -- 17:30 Computer Lab Session IV: MD and MC methods
Ray Atta-Fynn + Partha Biswas (UTA+USM)

June 5, 2019 Density functional theory

08:30-- 09:20 **Tutorial 8:** Introduction to density functional theory (DFT)
Eric Bylaska (PNNL)

09:20 -- 10:10 **Tutorial 9:** Density functional theory for disordered solids
David Drabold (Ohio University)

10:10 -- 10:20 Break

10:20 -- 11:10 **Tutorial 10:** Applications of DFT to solids: NWChem
Eric Bylaska (PNNL)

11:10 -- 12:00 **Tutorial 11:** Kinetic Monte Carlo (KMC) methods
De Nyago Tafen (National Energy Technology Laboratory (NETL))

12:00 -- 13:00 Lunch

13:00 -- 15:00 Computer Lab Session V: DFT methods
Eric Bylaska (PNNL)

15:00 – 15:15 Break

15:15 -- 17:30 Computer Lab Session VI: SIESTA
Drabold + Atta-Fynn (OU/UTA)

17:30 – 18:00 Conference group photo

18:00 – 20:00 Conference Dinner

June 6, 2019 Miscellaneous topics and Advanced modeling techniques

08:30 -- 09:20 **Tutorial 12:** Theory and simulation of lattice thermal conductivity of Solids
Jianjun Dong (Auburn University)

09:20 -- 10:10 **Tutorial 13:** Integrals and Integro-differential equations
Khin Maung (The University of Southern Mississippi)

10:10 -- 10:20 Break

10:20 -- 11:10 **Tutorial 14:** Advanced modeling techniques – I
Partha Biswas (University of Southern Mississippi)

11:10 -- 12:00 **Tutorial 15:** Advanced modeling techniques – II
Raymond Atta-Fynn (University of Texas at Arlington)

12:00 -- 13:00 Lunch

13:00 -- 15:00 Computer Lab Session VII: Advanced Techniques I + II
Raymond Atta-Fynn + Partha Biswas (UTA + USM)

15:00 – 15:15 Break
15:15 -- 17:30 Computer Lab Session VIII: Kinetic Monte Carlo
De Nyago Tafen (NETL)

June 7, 2019: HBCU Forum discussions and future collaborations

08:30 -- 09:30 Discussion among participants
Coordinator: Raymond Atta-Fynn (University of Texas Arlington)

09:30 – 10:00 Summer projects at the USM
Partha Biswas (The University of Southern Mississippi)

10:15 -- 10:45 Break + Documentation check for computer + Photo

10:45 -- 11:00 Summer projects at the USM
Khin Maung

11:00 -- 11:15 Project at UTA
Raymond Atta-Fynn (University of Texas Arlington)

11:15 -- 12:15 Problem assignment for evaluation
Partha Biswas/Raymond Atta-Fynn

12:00 – 13:00 Lunch

13:00 -- 17:00 Project completion and report submission + Program Survey

17:00 – 17:30 Award of certificates and closing ceremony