**A screenshot of a cell phone

Description automatically generated**

**Recent Developments in Computer Simulational Studies**

**in Condensed Matter Physics**

***Tentative Program of the 2025 – 38th Annual Workshop***

**Monday, February 24**

8:30 – 10:00 AM Registration in Room 321C of the Physics Building

9:00 - 10:00 AM Coffee, Tea and Pastries in 3rd floor CSP area

Informal discussion in Conference Room 322

10:00 – 10:05 AM **Anna Stenport,** Dean, Franklin College of Arts qnd Sciences

10:05 – 10:10 AM **Phillip Stancil,** DepartmentHead of Physics and Astronomy

10:10 – 10:20 AM **David P. Landau**, Director, Center for Simulational Physics

10:20 – 11:20 AM **Mohamed Laradji,** University of Memphis

"Lipid Membranes as a Tool for Self-Assembling Nanomaterials into Ordered Nanoclusters and Superlattices"

11:35 – 11:50 AM **Ying Wai Li,** Los Alamos National Laboratory

“Materials Inverse Design by Monte Carlo Tree Search and First Principles Calculations”

12:00 PM Lunch

2:00 – 3:00 PM **David Dahlbom**, Oak Ridge National Lab

“Generalizations of classical spin dynamics in the Sunny.jl project”

3:15 – 3:30 PM **Shan-Ho Tsai**, University of Georgia

“Phase diagram of a two-dimensional Q-state Potts model in an external field”

Coffee break

4:00 – 4:15 PM **Steven Hancock**, Johns Hopkins U. Applied Physics Lab

“Metropolis Sampling of Atomic Reconstruction of Twisted Bilayer Metal Dichalcogenide Models”

4:30 – 4:45 PM **Efstratios Manousakis,** Florida State University

“The random-phase-approximation based functional and its performance".

**A screenshot of a cell phone

Description automatically generated**

**Recent Developments in Computer Simulational Studies**

**in Condensed Matter Physics**

***Tentative Program of the 2025 – 38th Annual Workshop***

**Tuesday, February 25**

9:00 – 10:00 AM Coffee, Tea and Donuts in 3rd floor CSP area

Informal discussion in Conference Room 322

10:00 – 11:00 AM **Tsuyoshi Okubo,** University of Tokyo

“Tensor network approach to quantum spin liquid”

11:15 – 11:30 AM **Markus Eisenbach**, Oak Ridge National Laboratory

“First principles calculations of electric conductivity in complex materials”

11:45 – 12:00 PM **Aojie Xue,** University of Georgia

“Test of A Universality: First Order Transition in the Lebwohl-Lasher Model”

12:00 PM Lunch

2:00 – 3:00 PM **Achille Giacometti**, Universita' Ca' Foscari Venezia

“Phase behaviour and self-assembly properties of semiflexible polymers in solution ”

3:15 – 3:30 PM **Yong Wei**, University of North Georgia

“PDMD: Potential-free Data-driven Molecular Dynamics for Variable-sized Water Clusters (H2O)n ≤ 21”

Coffee break

4:00 – 4:15 PM **Shishir Bhusal,** University of Georgia

“Spatio-temporal Pattern Formation by the Biological Clock in *Neurospora Crassa*”

4:30 – 4:45 PM **Wolfhard Janke,** University of Leipzig

"Fast, hierarchical, and adaptive algorithm for Metropolis Monte Carlo simulations of long-range interactions”

**A screenshot of a cell phone

Description automatically generated**

**Recent Developments in Computer Simulational Studies**

**in Condensed Matter Physics**

***Tentative Program of the 2025 – 38th Annual Workshop***

**Wednesday, February 26**

9:00 – 10:00 AM Coffee, Tea and Donuts in 3rd floor CSP area

Informal discussion in Conference Room 322

10:00– 11:00 AM **Nima Karimitari,** University of South Carolina

“A Generalized Machine-learned Interatomic Potential for Chemical Reaction Pathways and Transition States”

11:15 – 11:30PM **Gabriel Bruno,** Universidade Federal de Minas Gerais

"Revealing the role of ripples in phonon modes for MoS2 and MoSe2: Insights from molecular dynamics and machine learning"

11:45AM Group Photo. (Outside the back entrance to the Physics Bldg.)

12:15 PMLunch

2:00 – 3:00 PM **Mariyi Fernandez-Serra,** Stony Brook State University

“Machine learning the exchange and correlation functional in DFT”

3:15 – 3:30 PM **Kipton Barros,** Los Alamos National Laboratory

“I have a new algorithm for the long-range Ising model; can ChatGPT help with prototyping?”

Coffee break

4:00 – 4:15 PM **Trinaanjan Datta,** Augusta University

“Dynamical phase transitions in the XY model: A Monte Carlo and mean-field theory study”

4:30 – 5:30 PM **Roundtable Discussion: Random Number Generation**

**Led by** **Panos Argyrakis,** University of Thessaloniki

6:00 – 8:00 PM **Reception** – Center for Simulational Physics Foyer

**A screenshot of a cell phone

Description automatically generated**

**Recent Developments in Computer Simulational Studies**

**in Condensed Matter Physics**

***Tentative Program of the 2025 – 38th Annual Workshop***

**Thursday, February 27**

9:00 – 10:00 AM Coffee, Tea and Donuts in 3rd floor CSP area

Informal discussion in Conference Room 322

10:00 – 11:00 AM **Oleksandra Kukharenko,** Max Planck Institute for Polymers

“Determining glass transition in polymer melts using machine learning”

11:15 – 11:30 AM **Aniket Bhattacharya,** University of Central Florida

“Probing dynamical heterogeneities in Intrinsically Disordered Proteins using Molecular dynamics, MC simulations, and Deep Learning”

11:45 – 12:00 PM **Alfred Farris**, Los Alamos National Lab

“Efficient method to determine the melting point from molecular dynamics simulations of liquids”

12:00 PM Lunch /Women’s Lunch

2:00 – 2:15 PM **Itay Hen,** University of Southern California

**“**Permutation matrix representation quantum Monte Carlo: A universal framework for simulating arbitrary quantum many-body systems”

2:30 – 2:45 PM **Maninder Kaur,** University of Georgia

“Can Machine Learning Truly Decode Phase Transitions? A Deep Dive into the Ising Model with Competing Interactions”

3:00 – 3:15pm **Manoi Kumar,** NISER Bhubaneswar

“Critical aspect on three-dimensional random-field Potts model”

Coffee

4:00 – 5:00 PM **Dept. Colloquium/Workshop Invited Talk** (Room 202)

**Thomas Vogel,** Los Alamos National Lab

“Confusing Neural Networks in Simulational Physics”

**A screenshot of a cell phone

Description automatically generated**

**Recent Developments in Computer Simulational Studies**

**in Condensed Matter Physics**

***Tentative Program of the 2025 – 38th Annual Workshop***

**Friday, February 28**

8:30 – 9:00 AM Coffee, Tea, and Donuts in 3rd floor new addition foyer

Informal discussion in Conference Room322

9:00 – 10:00 AM **Nobuyasu Ito,** RIKEN

“Application of evacuation simulations to Kobe city”

10:15 – 11:15 AM **Lukas Stezl,** University of Mainz

"Coarse-grained molecular dynamics simulations of protein phosphorylation in condensates"

11:30 – 11:45 AM **Binder Lecture:**

**Martin Weigel,** Technical University of Chemnitz

“Low-energy excitations in spin glasses”

12:00 PM **David Landau** Director, Center for Simulational Physics

Closing Remarks