Spring (2021) Leaders Meeting Agenda
Saturday, April 10

We will meet in one main Zoom session.
https://umsystem.zoom.us/j/96840364937?pwd=SlVSOGsxbW1iczdycDM4VXUvK0t4QT09
Meeting ID: 968 4036 4937
Passcode: 922637

Leaders will be emailed a link to a second private Zoom session for private discussion next week.

All times CDT

Saturday April 10:

10:00 am	Zoom session open for joining and visiting. Informal discussion
10:20 am	Paul Miceli welcome comments, brief status of the department for the spring semester Remarks by John Shumway
	Undergraduate presentations, 20 minutes each, including Q&A:
10:40 am	**Matthew Snyder** (Advisor Prof. Guang Bian) *"Monte Carlo Studies of Nontrivial Defect Boundaries in an Ising Model Magnet"*
11:00 am	**Rory Butler** (Advisor: Prof. Suchi Guha) "*Magnetic Field Dependence of the Optical Properties in Lead Halide Perovskites"*
	Graduate student presentations, 20 minutes each, including Q&A
11:20 am	**Payal Bhattacharya** (Advisor: Prof. Suchi Guha) "*Third Harmonic Generation in Lead Bromide Perovskites*"
11:40 pm	**Break** (leaders could choose to rank undergraduate presentations – private separate Zoom)
12:40 am	**Alex A. Daykin** (Advisor: Prof. Paul Miceli) "Hydrogenated Graphene: A Complicated Structure"
1:00 pm	**Ryan Smith** (Advisor: Prof. Ioan Kosztin) *"Energetics and Kinetics of Peptide-Lipid Membrane Interactions: A Molecular Dynamics Study"*
1:20 pm	**Alex Bretana** (Advisor: Prof. Wouter Montfrooij) *"The appearance of spontaneous disorder in disorder-free systems"*
1:40 pm	Break/ Leaders discussion on ranking student presentations (separate Zoom)

2:15 pm Student award presentations
2:30 pm Closing remarks
2:45 pm Adjourn

The Leaders private zoom room left active for their business meeting

Undergraduate Student Presentations

Speaker: **Matthew Snyder** (Advisor Prof. Guang Bian)

Title: *Monte Carlo Studies of Nontrivial Defect Boundaries in an Ising Model Magnet*

Abstract: We describe an approach of using Monte Carlo simulations to report the effects of various nontrivial configurations of a two-dimensional Ising model Magnet on select thermodynamic parameters. These configurations include a checkerboard pattern generated by introducing a finite number of defect lines, topological configurations such as a torus, Mobius strip, and Klein bottle, and a study of the finite size effect on a given configuration with a given number of defects. While each of these configurations has a well-defined ground state the system would frequently converge to a locally stable configuration with drastically different thermodynamic parameters. As such, we present a method using the Swendsen-Wang cluster Monte Carlo algorithm to drastically reduce the runtime for the system to converge while mitigating these locally stable convergence problems that appear throughout our configurations.

Speaker: **Rory Butler** (Advisor: Prof. Suchi Guha)

Title: **Magnetic Field Dependence of the Optical Properties in Lead Halide Perovskites**

Abstract: Lead halide perovskites are promising semiconductor materials usable in a wide range of optical technologies including photovoltaics and light-emitting devices. But the excitation and emission processes of these materials is part of ongoing debate and not well understood. The strong spin-orbit interaction in these materials has several ramifications in the optical properties. We examine the magnetic field dependence of the photoluminescence (PL) in $CsPbBr_3$. Along with an enhancement in the PL intensity, changes in the PL lifetimes are observed. Our results suggest that an applied magnetic field influences the population and behavior of triplet states in $CsPbBr_3$. These results are compared with a triplet-enhanced conjugated polymer. We further discuss our on-going efforts to enhance the capability of time-resolved PL measurements using an ultrafast laser system.

Graduate Student Presentations

Speaker: **Payal Bhattacharya** (Advisor: Prof. Suchi Guha)

Title: *Third Harmonic Generation in Lead Bromide Perovskites*

Abstract: Lead halide perovskites have garnered a lot of attention both in displays and photovoltaics. Along with their remarkable linear optical properties, these materials provide a testbed for exploring nonlinear optical properties. As in the case with several of the 3D lead halide perovskite systems, the underlying centrosymmetric crystal structure precludes the phenomenon of second harmonic generation. However, the third and higher-order harmonic generation are allowed. In this work, we probe the third harmonic generation (THG) from $CsPbBr_3$nanocrystals (NCs), synthesized via hot injection method, and compare it to the THG from $CsPbBr_3$ NCs with Ruddlesden-Popper planar faults (RP-$CsPbBr_3$), formed via post-synthetic fusion-growth. The THG from CsPbBr3 NCs is negligible compared with that of RP-$CsPbBr_3$ NCs within a wide range of femtosecond excitation wavelengths: 1100–1400 nm. The THG efficiency of a thin film of RP-$CsPbBr_3$ is found to be at least three times larger than the value from a single crystal of methylammonium lead bromide ($MAPbBr_3$). By comparing with $MAPbBr_3$, we obtain χ^3_{eff} for a thin film of RP-$CsPbBr_3$ to be of the order of $10^{-17}m^2V^{-2}$. This work opens up the potential of inorganic halide perovskite NCs with planar defects as a platform for a range of nonlinear optical applications.

Speaker: **Alex A. Daykin** (Advisor: Prof. Paul Miceli)

Title: Hydrogenated Graphene: A Complicated Structure

Abstract: Defects and functionalization can be used to modify graphene's physical properties such as changing its conductivity or inducing ferromagnetism, which is of interest for spintronics. One method of modifying graphene is attaching hydrogen to the surface of the carbon sheets during the graphene synthesis, which has been carried out on bulk graphene powders. While many interesting property changes have been observed in hydrogenated graphene, the research community has still not experimentally determined the atomic structure of these materials, particularly the locations of the hydrogen in the graphene lattice. In this work we utilize neutrons' sensitivity to hydrogen to show that the structure of these materials is more complex than the idealized picture predicted by theory that many researchers may assume.

Speaker: **Ryan Smith** (Advisor: Prof. Ioan Kosztin)

Title: *Energetics and Kinetics of Peptide-Lipid Membrane Interactions: A Molecular Dynamics Study*

Abstract: Quantitative characterization of the binding strength of peptides to lipid bilayers is crucial in understanding the molecular mechanism of cellular processes triggered by peptide-lipid interactions. In general, single molecule methods, such as high precision AFM based dynamic force spectroscopy, can be used to measure the dissociation force distribution, *P*(*F*), and the corresponding force dependent dissociation rate, *k*(*F*), of individual peptides bound to a lipid bilayer. However, the interpretation of the results requires extensive theoretical and computational modeling that implies the knowledge of the free energy profile (potential of mean force or PMF) of the system, $U(z)$, as a function of the separation, z, between peptide and membrane surface. To this end, we have used all atom MD simulations, to calculate the PMF of three representative Wimley-White pentapeptides (pX=Ac-WLXLL, with guest residues X=R,I and L) interacting with two different lipid bilayers (zwitterionic POPC and charged POPG). The PMF, $U(z_W)$, as a function of the distance, z_W, between the residue W and the plane of the membrane, was calculated by using the equilibrium *umbrella-sampling* method. The values of the activation energy (free energy barrier), ΔU_0, and activation length, Δx_0, extracted from the PMFs appear to be comparable to previous experimental and computational studies, and thus can be used to interpret and predict $P(F)$ and $k(F)$ from AFM measurements.

Speaker: **Alex Bretana** (Advisor: Prof. Wouter Montfrooij)

Title: *The appearance of spontaneous disorder in disorder-free systems*

Abstract: When modeling phase transitions in stoichiometric, disorder-free systems, theories naturally do not include the role of disorder. However, we show that when systems are prepared to be on the verge of ordering at zero kelvin, so the so-called quantum critical systems, that this assumption breaks down in disorder-free systems. In fact, we find that omnipresent quantum mechanical effects cause a spontaneous fragmentation of the magnetic lattice and that the response of the system near the phase transition is dominated by this fragmentation. The implications of these findings are far-reaching as it essentially invalidates the current theories of what drives quantum phase transitions.