

(Special Seminar)



Probing non-equilibrium dynamics in complex materials using ab-initio-based approaches

Dr. Sangeeta Rajpurohit Lawrence Berkeley National Laboratory

spin, and lattice degrees of freedom The interplay between charge, in complex materials under external stimuli gives rise to several fascinating phenomena, such as photo-induced phase transitions, non-linear optical effects, and transient 'hidden' phases. Theoretically, studying these processes is a challenging task that requires methods that can cover timescales of various active degrees of freedom. The complex interactions and correlated processes in materials add further complication. In this talk, I will discuss the microscopic modeling of the relaxation dynamics of complex oxides exhibiting long-range charge and orbital orders. The photo-induced dynamics in these systems are highly selective depending on the light-pulse intensity and polarization. I will provide insight into possible and lattice-assisted relaxation mechanisms. Additionally, I will present simulation results spindemonstrating how optical excitations can serve as a powerful tool to control spin-splitting gaps in the newly discovered class of magnetic materials known as altermagnets. In the second part, I will discuss the impact of interactions and guasiparticle dynamics on non-linear optical properties. I will present real-time dynamics of photocurrent generation in ferroelectrics, emphasizing the role of spin- and phonon-driven ballistic photocurrents alongside the shift current.

Monday, February 3, at 10:30 AM, CSP Conference Room 322, Physics Building

Local Contact: Prof. Y. Abate, yohannes.abate@uga.edu