March 7th, 2022 10:00 AM
QED & Materials seminar
Mukhtar Lawan

Title
"Transient Absorption Spectroscopy to Investigate Bandgap Dynamics in Monolayer Hexagonal Boron Nitride (hBN)"

Abstract
Two-dimensional (2D) Hexagonal Boron Nitride (h-BN) is an insulator that has polar covalent B-N bond. Both monolayer and bilayer (h-BN) emerge as an optoelectronic material, which can be used as photodetectors and for photocatalysis. Herein, we performed calculation for Transient absorption spectroscopy (TAS) for monolayer (h-BN) using linear, collinear and bicircular pump pulses, modelling the dynamics with Time Dependent Density Functional Theory (TDDFT) numerical pump probe simulation as implemented in the octopus code. The pump probe measurement is numerically simulated by solving the Time dependent Kohn-Shams (TDKS) equation using the pump and probe field as external fields.