Towards Machine Learning Plasmon Driven Photocatalysis and Spectroscopy

Sajal Kumar Giri

Department of Chemistry, Northwestern University, Evanston, USA

Abstract:

Photocatalysis is a topic of significant interest in applications to solar fuels, sensing devices, and organic synthesis. In the last 15-20 years, the use of plasmonic nanoparticles (Au, Ag, Cu, and Al) has become a major activity within the photocatalysis field. In this talk, I will discuss whether we can integrate machine learning methods to circumvent the existing theoretical challenges in studying plasmon driven chemical reactions and spectroscopy. A variety of reactions have been considered, ranging from very simple processes like the dissociation of H_2, the formation of negative ions of molecules adsorbed on the particle surfaces, and reactions important in energy science such as CO2 reduction, and water splitting.