CHYN MEETS HARBOR

Materials with Atomic Precision

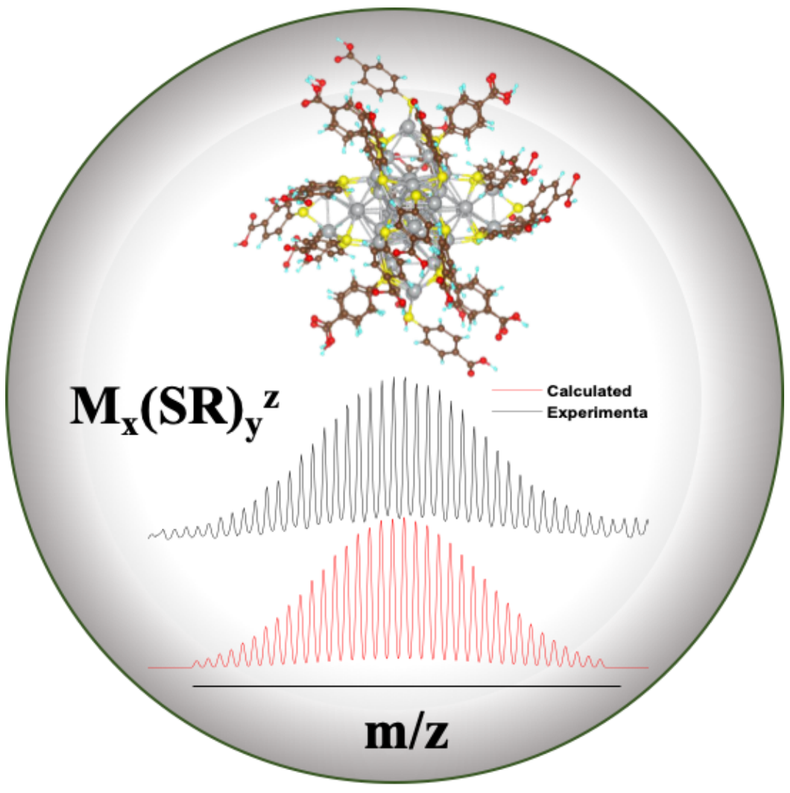
Dr. Indranath Chakraborty

Ab initio calculations of defects in semiconductors and their optical properties

Walter Pfäffle

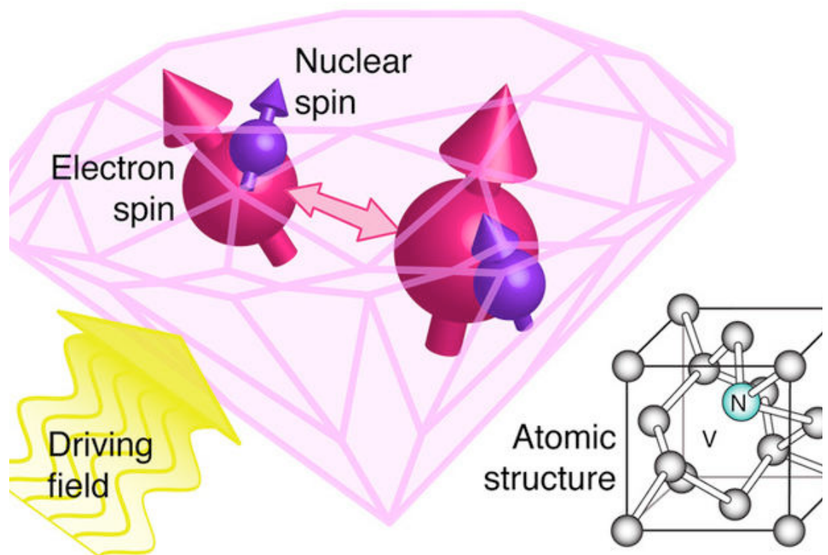
Abstract Talk 1: Noble metal nanoclusters (NCs) are molecular entities composed of atomically precise cores with well-defined ligand shells. They have distinctly different properties than the corresponding plasmonic nanoparticles and bulk materials**.** Surface atoms play a significant role in determining the properties of nanosystems. As the number of such atoms is large in NCs, they show unique optical and photophysical properties due to their tiny core size (1-2 nm).

Ligands can also add new properties in such NCs. Their typical photoluminescence quantum yield is several orders of magnitude higher than the corresponding nanoparticles. Potential applications of this new class of materials are numerous, but the field is just emerging. Many exciting properties have not been explored yet. This talk will give an in-depth understanding of this fascinating class of material (including synthesis, characterization, structure, properties, and applications). Along with that, the talk will also highlight how the understanding of this emerging material can be translated into academic curriculum in terms of a laboratory experiment.



Abstract Talk 2: We present a method to derive atomic effective potentials for defects in semiconductors (AEPs) based on the total screened potentials calculated using density functional theory that involves no free parameters and features a robust procedure for achieving a dense G-space sampling

We take advantage of the fundamentally short-ranged nature of impurity-induced potential changes and demonstrate that impurity potentials obtained using the self-consistently calculated potentials for small supercells can be accurately applied in non-self- consistent calculations for different geometries and substantially larger systems. This approach allows an accurate treatment of impurity problems free from the significant restrictions usually associated with finite supercell. In a next step a screened configuration interaction calculation is able to accurately treat highly correlated electron spins localized around semiconductor defects. Impurity cal- culations for substitutional Mn, group-IV acceptors in GaAs and the negatively charged nitrogen vacancy defect in Diamond are presented.



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15.12.2020
1:15 pm | Zoom

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