Professor Ray’s research focuses on acquiring knowledge from nature about
the principles governing reactivities in biological systems that employ com-
mon transition metals like copper, iron, manganese, etc. In order to interpret on
a molecular level the data of metallopro-
teins and metalloenzymes, acquired by
various physical methods, low-molecu-
lar weight synthetic model compounds
are necessary as reference substances.
His group focuses on synthesizing mod-
el complexes (both functional and struc-
tural) for monooxygenase and oxidase
enzymes using newly designed chelat-
ing ligands. A battery of spectroscopic
techniques, which cover more than 10
orders of magnitude in photon energy,
characterizes the complexes. Differ-
ent energy regions provide different
complimentary insights into the prop-
erties of the complexes under study.
By choosing the right combination of
methods coupled with the ligand field
and molecular orbital theories, a definite
picture about the electronic structure of
the model complexes can be obtained,
furthers understanding on the actual
enzymatic systems.

Information:
https://z.umn.edu/RayKallol

Small Molecule Activations
at Transitional Metal Centers:
Structure-Function Correlations

Professor Kallol Ray
Department of Chemistry
Humboldt-Universität zu Berlin

Small molecule activation constitutes one of the main frontiers
of inorganic and organometallic chemistry, with much effort
directed towards the development of new processes for the
selective and sustainable transformation of abundant small
molecules such as dioxygen (O₂), water (H₂O), hydrogen perox-
ide (H₂O₂) or protons (H⁺) into high-value chemical feedstocks
and energy resources. Because nature mostly uses metal ions
to activate these relatively inert molecules and modulate their
reactivity, much inspiration for the field has come from bioin-
organic chemistry. This talk will focus on some of the recent
highlights from our group on homogenously catalyzed bioin-
spired activation of small molecules, as well as stoichiometric
reactions that further our understanding towards such ends. It
will cover many aspects of small molecule activation including:
organometallic chemistry, spectroscopy, synthesis, and detailed
mechanistic studies involving trapping of reactive intermedi-
ates. The demonstrated examples will help to emphasize the
continuous effort of our group in uncovering the structure-
reactivity relationships of biomimetic model complexes, which
may allow vital insights into the prerequisites necessary for the
design of efficient catalysts for the selective functionalization of
unactivated C–H bonds, O₂/H₂O/H₂O₂ activations, or H⁺ reduc-
tions by using cheap and readily available first-row transition
metals under ambient conditions.