Research in our group revolves around applying spectroscopic techniques to answer questions about iron coordination complexes and their role in biochemical processes. Students learn how to use Mössbauer spectroscopy to answer questions that cannot be answered by traditional spectroscopic methods. For example, one of our recent papers addressed the Mössbauer spectroscopy of bimetallic spin-coupled assemblies which are also electrocatalysts for hydrogen generation. (Link to our 2019 Inorganic Chemistry paper: 10.1021/acs.inorgchem.9b00746)

Currently some of the questions we ask fall in two general directions.

(1) Elucidation with Mössbauer spectroscopy of the structure of certain iron centers involved in cellular iron protein biosynthesis and cellular iron trafficking. All cells need to maintain iron homeostasis, a multitasking feat done employing a variety of proteins and regulatory mechanisms that are not understood. We ask what type of iron centers are found in these proteins how are these iron centers performing their functions.

(2) Determination with Mössbauer spectroscopy of spin couplings and electronic ground states in complexes involved in catalytic processes of biological relevance. Biological oxidation is a central process in the carbon geochemical cycle. Bacteria have specialized degradation pathways for classes of chemical structures, which have evolved in response to environmental demands. A particular class of enzymes are the non-haem (non-heme) mononuclear iron oxygenases. We aim to elucidate with Mössbauer spectroscopy the types of reactive intermediates that are necessary to oxidize certain substrates.

(3) Elucidation of the electronic ground states and determination of hyperfine interactions using Mössbauer spectroscopy, for bio-inspired iron complexes that challenge our understanding of bonding and electronic structure.

Although $^{57}$Fe-Mössbauer spectroscopy is specialized to iron, given iron's status as the most abundant transition metal in the Earth's crust, the number of potential systems to study is limited only by our time and ability to focus on the proper questions and to figure out the correct answers. When the questions are about electronic structure, our students must first learn how to plan the conditions for the collection of the spectra that are optimal for the sample at hand. As it is the case with most spectroscopic techniques, good Mössbauer spectra are not trivial to collect and interpret. Because spectroscopy is expensive and it must be precise and accurate, the equipment has to be carefully calibrated and maintained. Thus, students spend time with Dr. Popescu collecting calibrations, calculating calibration parameters, running standards and also fitting spectra while they are still collecting, so as to plan the next experimental conditions. Our lab typically does spectroscopy at temperatures between 5 and 280 K and we work with other labs who collaborate with us because the questions we ask are essential for their research. In order to obtain high-quality spectra, our students also learn about the sample preparation and how to chemically manipulate and modify samples.

Iron has been used by living systems to construct protein and enzyme active sites of exquisite complexity, since the beginning of life on Earth. A few examples of iron proteins are iron-sulfur proteins, heme and non-heme enzymes, which can be found in organisms from bacteria to mammals. There is great interest in the mechanisms of these proteins, motivated by their importance for life processes such as respiration, biological oxidation and aspects of mammalian iron homeostasis, to name only a few. On the other hand, chemists are also interested in the mechanisms of iron enzymes, because nature can be an inspiration for
chemists in their effort to design iron-based molecular catalysts for sustainable degradation of pollutants and other important processes.

Mössbauer spectroscopy is widely used for the identification of oxidation state, spin state and coordination sphere, in iron compounds. However, in our lab, we are interested in more than simply collecting parameters, rather we are contributing spectroscopic and structural insight in the mechanism of iron proteins and bio-inspired catalysts. Sometimes digging into a Mössbauer spectrum can uncover some unusual features, which—although initially appreciated only by the spectroscopist—lead to insights into larger questions, such as cluster conversion, electronic structure of a short-lived intermediate, or mechanistic steps that were not previously hypothesized. Being able to figure out these latter questions, which are appreciated by the larger community of biochemists and chemists, highlights the importance of Mössbauer spectroscopy and motivates the community to seek out collaboration with us.