Semiconductor nanocrystals are tiny particles which can be relatively easily synthesized in colloids. Their diameters are between 2 and 8 nanometers, i.e., 10000 times smaller than hair breadth. The size determines their properties and the size can be tuned by changing the reaction time. In particular, in this way scientists can engineer the color of the light these nanocrystals absorb and the color of light they emit. Easy solution processability and spectral tunability make nanocrystals exciting for many applications ranging from displays, via solar cells, to applications in medicine. However, the compounds whose properties are best understood are cadmium selenide and lead sulphide. These compounds contain highly toxic cadmium and lead ions and their use in industry is heavily restricted by international regulations. It is therefore necessary to develop alternative materials and learn how to engineer their properties toward applications.

In this project we will synthesize and investigate ternary nanocrystals — a class of nanomaterials described by a chemical formula ABX_2, where A is usually copper or silver, B is indium, gallium, aluminium or iron, and X (in the case of the planned studies) is sulfur. ABX_2 nanocrystals are thus made of non-toxic and Earth abundant elements, which makes them ideal for real-world applications. However, the understanding of optical properties of this class of materials is relatively underdeveloped. Even for the most widely studied $CuInS_2$ nanocrystals, the mechanism of light emission is a subject of a heated debate.

Within this project we will perform comprehensive studies of optical properties of ABX_2 nanocrystals to discover what makes them emit light. To this end, we will investigate the dynamics of photoexcited electrons, study the optical properties at liquid helium temperatures, and investigate light signals emitted by single nanocrystals. These studies will require to use ultrafast lasers — emitting light pulses as short as 1 billionth of a second and ultrasensitive detectors — capable of registering arrival times of single photons. Our experiments will be aided by theoretical calculations, which will allow us to compute the energy spectra by building the modelled nanocrystals atom by atom. These calculations will be carried out with the use of large, high performance computers. Combining the theoretical and experimental investigations will show us how the size, structure, chemical composition, and the environment impact the optical properties of ABX_2 nanocrystals. As a result, we will be able to present strategies for optimization of the optical properties for particular device applications.

Indeed, we will use this knowledge to engineer the way the ABX_2 nanocrystals absorb light. Since the demand for electricity is dramatically increasing worldwide, it is imperative to develop new, safe, and efficient sources of energy. Present day solar cells convert energy from sunlight to electricity quite inefficiently: only photons with specific energy can be used to produce electric current. In this project, we will investigate the possibility of adapting the solar spectrum to match this specific energy value. Namely, we will add small amounts of lanthanide ions to the ABX_2 crystal structure. These ions can up-shift or down-shift the energy of photons. We will determine the efficiency of this process to understand whether it is a viable route toward improving solar cell efficiency.

The proposed studies concern a relatively unknown class of materials. It is reasonable to expect that the results obtained within this project will resonate with the community investigating colloidal nanocrystals and pave the way toward new application ideas.