

Effect of Hydrostatic Pressure and Temperature on Polarons, Excitons, and Phase Transitions in Selected Hybrid Organic-Inorganic Perovskites

Hydrostatic pressure is one of the factors that can significantly change the optical, electrical and structural properties of crystals. At sufficiently high hydrostatic pressure, which can be achieved in diamond anvils, it is possible to spectrally retune the light emission from the crystal, a non-conducting crystal can be "converted" into a conducting metal, or a structural phase change can be achieved, i.e. the arrangement of atoms in the crystal can be changed.

In this project, we plan to conduct comprehensive optical, electrical, and structural studies at high hydrostatic pressures (up to ~10 GPa) for hybrid organic-inorganic perovskites. These types of crystals are very suitable for this type of research because of their high softness compared to other semiconductor crystals such as group III-V or II-VI semiconductors. Due to their high softness, free charges in perovskite crystals disturb the arrangement of atoms, i.e. they attract (or repel) atoms towards (from) each other depending on the charge, and therefore instead of quasiparticles such as electrons and holes with their characteristic effective masses, negative and positive polarons may appear, i.e. electrons (holes) coupled with phonons (quasiparticles that describe the vibrations of atoms), and these are characterized by much larger effective masses. As a consequence, such quasiparticles as excitons (i.e. Coulomb-bound electrons and holes) can be very different because both free carriers (electrons and holes) and negative/positive polarons can participate in their formation.

We hypothesize that hydrostatic pressure will affect the polaron formation energies in the studied crystals, and thus will affect the spectral position of excitons in emission and absorption. To investigate this, complementary emission measurements (photoluminescence) and absorption measurements (reflection measurements) as a function of hydrostatic pressure performed at low temperatures are necessary because excitons are clearly visible in the PL and R spectra only at low temperatures. The observed changes in the PL and R spectra may be related to the creation/disappearance of polarons, the appearance of point defects or structural phase transitions. In order to be certain about the absence or presence of a structural phase transition at a given pressure, we plan parallel structural studies using the XRD and Raman methods. Such studies will allow us to construct full P-T phase diagrams for the studied perovskites.

We expect that the result of this project will be understanding the mechanism of formation of such quasiparticles as polarons and excitons in relatively soft matter, i.e. hybrid organic-inorganic perovskites. In addition, the result of the project will be the development of research methods, i.e. measurements at high hydrostatic pressure at low temperatures. This is a particular challenge for XRD measurements and therefore there are not many literature reports on phase transitions in perovskites under pressure at low temperatures.