

# CHYN MEETS HARBOR

Carrier dynamics in colloidal mid-infrared HgTe quantum dots

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Predicting the Charge Transport Properties of Molecular Junctions

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**Abstract Talk 1:** Colloidal quantum dots (QDs) are semiconductor particles smaller than the respective Bohr radius. This reduction in size leads to drastic changes in material properties, such as the quantization of energy levels. Especially the increase in band-gap due to the localization energy allows to tune emission and absorption frequencies with particle size.

Consequently, colloidal nanocrystals present an alternative to epitaxially grown alloys for infrared (IR) applications, and the field of quantum dot based IR sensors and emitters is rapidly evolving. Additionally to these well understood changes in static properties, the carrier dynamics in QDs vastly differ from their bulk counterpart. In this talk, I will discuss the underlying physical principles as well as results from carrier dynamics in colloidal HgTe QDs studied by femtosecond infrared pump-probe spectroscopy.

**Abstract Talk 2:** Electron transport through nanoscopic objects from transport phenomena in, e.g., bulk materials. Small changes of a molecule can lead to large changes of its conductance caused by for example quantum interference. Measuring the transport properties of molecules is often done using scanning tunneling microscopy or a mechanically-controlled break junction setup.

In such systems, the molecules are subjected to mechanical forces, which (in addition to vibrations) change their structure and in that way the transport properties. Modelling such an experimental scenario can unveil the underlying physics and properties of a molecule of interest, but is a computationally demanding task: Even though the dynamics of the system can be captured with Molecular Dynamics (MD) simulations, a huge number of transport calculations have to be performed on top. In this talk, I will give an overview about my latest attempts to predict the transport properties of a molecule using machine learning approaches. This can significantly cut the computational time for the transport properties and also point to some underlying principles or reoccurring structure in the data.

