Dr. Yonatan Dubi - **Synopsis of research**

Motivation

Understanding the behavior of complicated systems at the nano-scale, and specifically how energy is transmitteed in nano-scale systems, is my major research theme. From a scientiffic point of view, these problems are perfect for a theorist, since they are very rich (and difficult), and include elements of non-equilibrium dynamics, electron correlation, molecule-surface interactions, fluctuations, electron-phonon interactions and more. However, studying these problems hold an additional bonus, since besides the scientiffic satisfaction, the succesfull research can be into improving our understanding of how energy flows and is converted in nano-scale systems, which may lead to future developments in the field of nanoscale energy conversion technology, which is considered one of the promising routes for overcoming the energy challenges our society is facing.

1. Thermoelectric effects in nano-scale junctions

The thermo-electric (TE) effect is the convertion a temperature gradient into an electric potential, a property which may be beneficial for future energy technology. Theory indicates thas molecular systems (i.e. Metal-molecule-metal junctions) can become superior thermoelectric converters and the thermoelectric response of a single-molecule junction have been measured in a set of impressive experiments. However, several of the experimental observations, including the value of the Seebeck coefficient and the observed large fluctuations, remain un-explined. My research is aimed at understanding the TE response of molecular junctions under various conditions, including the effects of junction geometry and contacts, presence of external fields (magnetic, microwave), optical excitations. The main goal is to understand how energy is transported in molecular junctiond, and how it can be controlled and manipulated with external means.

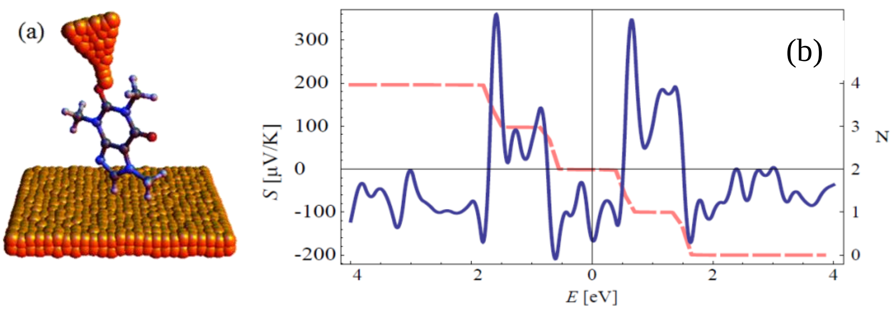

Fig. 1: (a) an example for a single-molecule junction. (b) The Seebeck coefficient of a molecular junction as a function of gate voltage, calculated using a method developed in my group.

2. Thermal transport in DNA nano-junctions

The DNA molecule is a key building-block of life. Thus, understanding the physical mechanisms which govern its behavior has become a great challenge. Specifically, understanding the denaturation transition of DNA (the seperation of the double-strand molecule into two single strands) is of great interest. My research is focused in understanding how energy flows through DNA nano-junctions as the DNA crosses the denaturation transition. The determination of the energy flow (via, e.g. the thermal conductance) has consequences to our understanding of DNA dynamics and the relaxation processes in DNA, to the way we model DNA in simulations, and for using DNA as a nano-technology template for future devices such as nano-scale thermal switches.

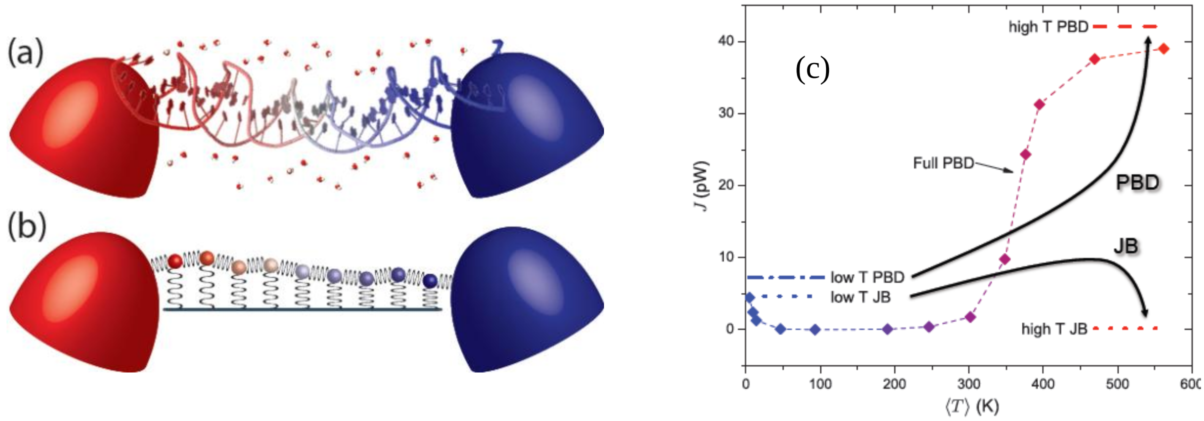

Fig.2: (a) A DNA nano-junction between two electrodes held at different temperatures. (b) A schematic representation of the models we employ to describe DNA. (c) thermal current of a DNA nano-junction as a function of energy, demonstrating unusual thermal switching behavior of DNA as it crosses the denaturation transmition – the seperation of the double strands into two single strands.

3. Electronic properties of Heay-Fermion materials

Understanding how interactions between localized and conduction electrons affect (or indeed determine) the electronic properties of complex materials have been a top issue in material sciecne. The topic has been revitalized in recent years, as new and ever-more sophisticated experimental tools have been introduced to strongly correlated materials on local scales, such as scanning tunneling spectroscopy. My research interest is in understanding the interplay between the global electronic structure and local nano-scale characteristics, i.e. how the electronic correlations affect the local STM images, and vice versa – how nano-scale features (such as disorder) are manifested in macro-scale measurements. Understanding these inter-relations is a substantial step towards the interpertation of nano-scale measurements in this important class of materials. This is becoming an important tool in understanding and identifying their properties, bringin us closer to the goal of “materials by design” – the design of materials with specific electronic properties.

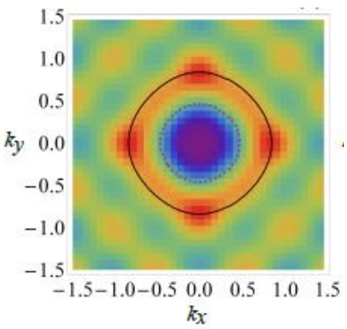

Fig.3: Local density of states and quasi-particle response of a hybridized heavy Fermion system with a nano-scale impurity.