# Turan Birol -Abstract

## Transparent Conducting Oxides and Hund's Metallicity in V-Nb Double Perovskites

Increasing reproducibility of first principles methods and availability of higher computer power made first principles calculations an integral part of solid state physics and materials science. Not only is it now possible to support and reproduce experimental observations ab initio, but it is also common to solve the inverse band structure problem to perform materials by design, i.e. to predict yet-to-be-synthesized compounds with desired electronic functionalities.

In this talk I am going to discuss some of my group's recent efforts to perform correlated materials design, and more specifically, design a transition metal oxide that is both metallic and transparent in the visible spectrum. Vanadate perovskites such as SrVO3 have been proposed for this application, and it was shown that the electronic correlations is essential for their optical transparency. Reproducing these electronic correlations require theoretical tools that go beyond the commonly used workhorse of materials simulations, the density functional theory (DFT). After a brief introduction of one such method, the Dynamical Mean Field Theory (DMFT), I will explore how DFT+DMFT can be used to design novel compounds that can be used as transparent conductors. Specific examples will include vanadates and niobates, and their double perovskites which turn out to be so-called Hund's metals. I will discuss how minor crystal structural details, and their interplay with the electronic structure, is very important in determining where these materials reside in the phase diagram. I'll conclude by a discussion on the effect of cation order in these compounds.