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Understanding the Metal-Insulator Transition in Certain Metal-Oxides

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Metal-Insulator Transitions of V_2O_3, VO_2, and Ti_2O_3

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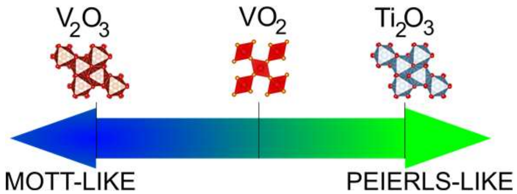
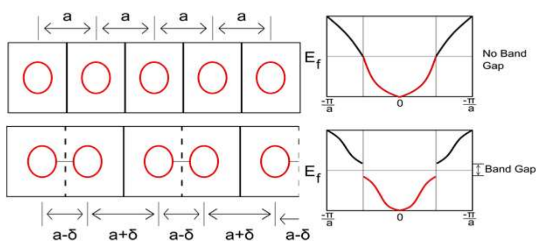


Transition Metal Oxides which undergo temperature dependent metal to insulator transitions fall onto a spectrum denoting the relative importance of electron correlation effects vs. structural distortions, and the transition is always driven by a combination of these mechanisms.

Ideal Peierl's transitions are driven by electron-localization brought about from structural deformation of 1-D ion chains. This leads to a doubling of the unit cell used to describe the crystal structure, and a subsequent band gap then forming.[2] Even materials with Corundum crystal structures such as Ti_2O_3 with no such obvious 1-D chain undergo a local distortion and dimer formation[4], making them quasi-peierl's transitions.

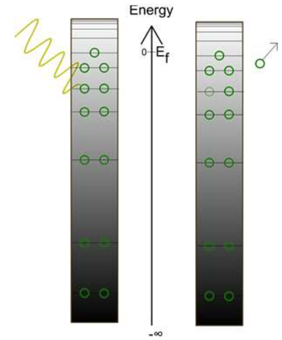


INTRODUCTION

Correlated metal oxides exhibit unique electronic properties which make them useful in novel electronic devices. V_2O_3, VO_2, and Ti_2O_3 specifically all experience a temperature-dependent metal to insulator transition (MIT), driven by a combination of structural distortions (Peierl's distortions) and electron-correlation effects (Mott transitions).

METHODOLOGY

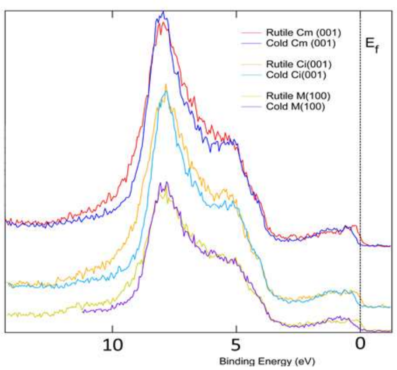
The main techniques we used (XPS, HAXPES, and XSW) all rely on the application of the photoelectric effect to measure the electronic structure of the material to probe the occupied electronic states.
The incident x-rays excite bound electrons in our material system, and the energy of these outgoing photoelectrons gives us information of the electronic property of the material.



Schematic of the Photoelectric Effect.

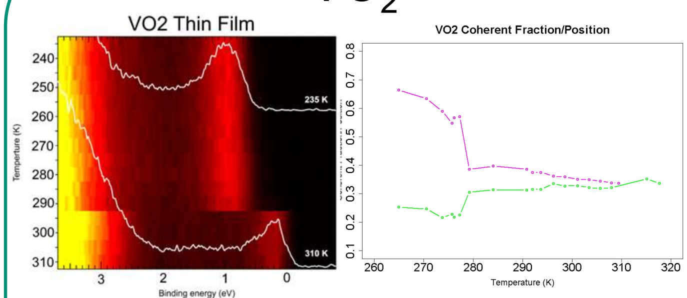
V_2O_3

Valence Band spectra of V2O3 thin films on multiple substrates providing epitaxial strain. We still see the expected MIT across all tested strain orientations.



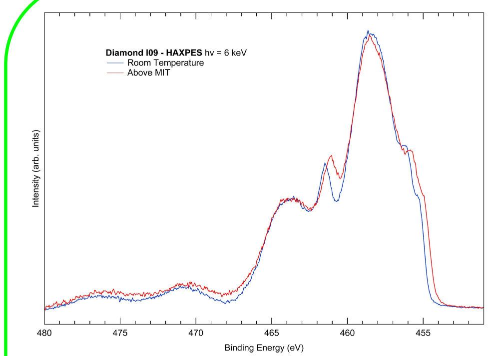
V_2O_3 was first used as an example of the quintessential Mott Transition before it was show to also have a structural phase transition as well.[1] Now there is an ongoing effort to find the effect of strain on the system's electronic structure.

VO_2



Rigorous study of VO2's MIT and structural phase transition (SPT) through the use of X-Ray Standing Waves shows the simultaneity of these first order transitions within our experimental limits,[5] which is contrary to other reports claiming to see a "decoupled" MIT and SPT.

Ti_2O_3



Ti2O3 was known to be a Peierl's transition[2], however we are able to see what is hypothesized to be a screened state in the Ti2p spectra, indicating the existence of some electron correlation effects present[6].

Techniques

X-ray Photoelectron Spectroscopy (XPS):
XPS applies the principle of Photoemission with x-rays to probe the electronic structure of materials.

HArd X-ray PhotoElectron Spectroscopy (HAXPES):
HAXPES applies the principle of Photoemission with high-energy x-rays to probe the electronic structure of materials and can gather information from deeper within the bulk of the sample, as well as from deeper core levels.

X-ray Absorption Spectroscopy (XAS):
XAS uses X-rays to measure the Partial Density of States.

X-ray Standing Waves (XSW):
XSW uses x-rays to simultaneously measure the structural and electronic properties of highly-ordered material systems.

National Synchrotron Light Source II (NSLS II) 7-ID-2 beamline. This light source provides X-Rays at energies which are inaccessible for typical lab-based techniques, allowing for more nuanced measurements.

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