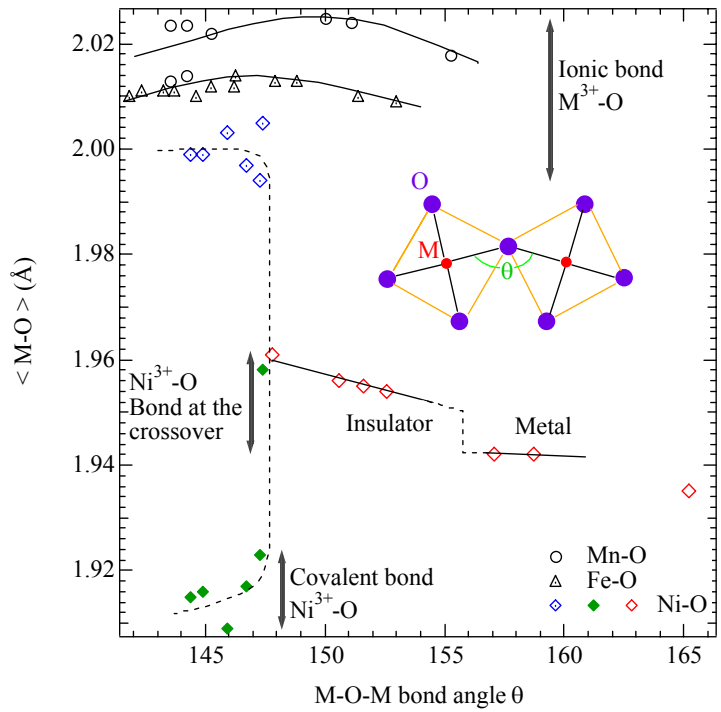
Orbital Order and Bond-Length Fluctuations in Narrow-Band Oxides

John B. Goodenough, University of Texas, DMR-0132282

Identification of vibronic bonding

The vibronic bonding introduces a strong electron-lattice coupling that results in unusual physical properties. In oxides, this new bonding occurs where bridging oxygen atoms oscillate perpendicular to the bond axis in a flat bond potential at a crossover from magnetic insulator to metallic conductor. The <Ni-O> bond lengths of the $RNiO_3$ family distinguish vibronic bonding in the Ni-O-Ni bond-angle range $148^\circ < \theta < 160^\circ$ from covalent and ionic bonding ($\theta < 148^\circ$) and metallic bonding ($\theta > 165^\circ$)



$RNiO_3$ family (R= Rare Earth) has Ni-O bond length which are clearly separated into four groups. The electronic bandwidth is adjusted by the M-O-M bond angle θ. The RMO_3 (M=Fe, Mn) shown for comparison have only ionic M-O bonds.

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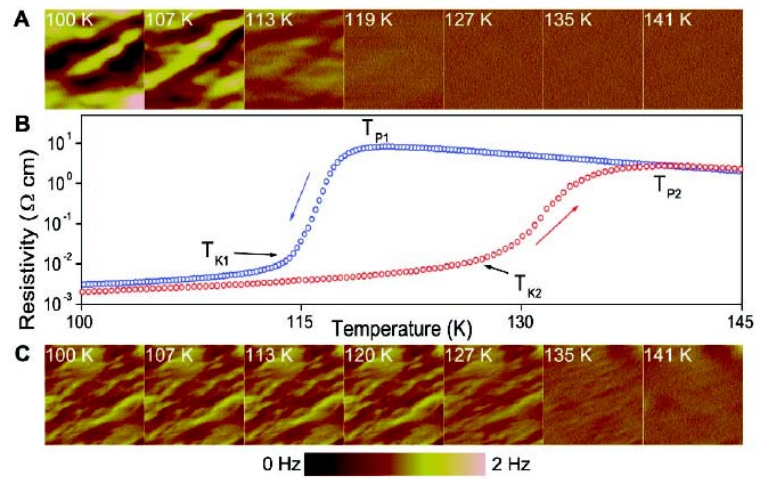
Education and Outreach:

The major research achievements have been introduced to the PI's graduate class " Localized to Itinerant electronic transitions in solids".

Four graduate students are presently involved in the project.

Plenary talks are given at international conferences each year.

The concept of a vibronic electronic state at the crossover from localized to itinerant electrons has been used to interpret the colossal magnetoresistance phenomenon, high-T_c superconductivity, and other unusual transport properties in metallic oxides.



The image of magnetic force microscope on a $La_{0.33}Pr_{0.34}Ca_{0.33}MnO_3$ film along with the temperature dependence of resistivity. The magnetoresistance effect is enhanced significantly at the transition where there is phase segregation into microdomains as shown from the image.

Cited from *Science* **298**, 805 (2002)