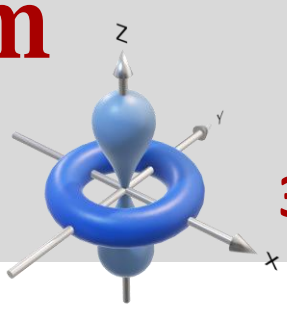
Department of Physics Colloquium

April 5, 2021 **3:00 PM**



Emergent phenomena in correlated complex oxides

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Complex oxides exhibit a wide range of exotic phenomena including metal-insulator transition, colossal magnetoresistance and high-temperature super-conductivity due to strong correlation effects arising from the d-orbital of transition metal ions. In this talk, we discuss two particular examples. The first example is $(SrRuO_3)_1/(SrTiO_3)_N$ superlattices in which the Ru magnetic anisotropy changes from two-fold along ⟨001⟩ axis ($\boldsymbol{N<3}$) to eightfold along ⟨111⟩ axis ($\boldsymbol{N\geq 3}$) [1]. Our first-principles calculations show that increasing the thickness of $SrTiO_3$ layers enhances the correlation effects on Ru, which induces a metal-insulator transition and a new orbital ordering. It is precisely this new orbital ordering that changes the underlying spin-orbit interaction and reorients the Ru magnetic easy axis. The second example is infinite-layer nickelates $R NiO_2$ (R is rare-earth elements) in which unconventional superconductivity has recently been discovered upon hole doping. We combine density-functional-theory and dynamical-mean-field-theory calculations to show [2] that there is a strong hybridization between correlated Ni-d orbitals and itinerant electrons in the rare-earth spacer layer. This makes the electronic structure of $R NiO_2$ distinct from that of superconducting infinite-layer cuprates $CaCuO_2$. As a consequence of hybridization, our calculations find that itinerant electrons screen the local moment on Ni site and increase the critical U_{Ni} that is needed to stabilize antiferromagnetic ordering. The results imply that the superconductivity observed in $R NiO_2$ does not emerge from a doped Mott insulator as in cuprates.

[1] Z. Cui, A. J. Grutter, H. Zhou, H. Cao, Y. Dong, D. A. Gilbert, Y. Liu, J. Ma, Z. Hu, J. Guo, E. Arenholz, H. Chen*, X. Zhai*, Y. Lu, *Science Advances* **6** eaay0114 (2020).

[2] Y. Gu, S. Zhu, X. Wang, J. Hu and H. Chen*, *Communications Physics* **3** 84 (2020).

All colloquia will be held via Zoom. Link to the Zoom session will be provided via email and Canvas