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Orbital-selective Mott transition in $Sr_2Mn_3As_2O_2$ VAIDEESH LOGANATHAN, ANDRIY NEVIDOMSKYY, Rice Univ — $Sr_2Mn_3As_2O_2$ is a layered material composed of alternating cuprate-like MnO_2 layers and MnAs layers similar to iron pnictides [1]. Recent neutron-scattering measurements have revealed a quasi-2D Neel-AF order in the MnO_2 layer, along with a G-type AFM order in the MnAs layer. To better understand the experimental findings, we have performed first-principles DFT+U calculations to explore the electronic structure in this material. We find the MnAs layer to be a simple Slater insulator due to the AF ordering. The MnO layer displays more correlated electron behavior that affects the transport properties. We observe a Mott transition in the MnO layer arising from the $d_{x^2-y^2}$ orbitals, reminiscent of cuprate superconductors. To study the layer- and orbital-selective Mott transition, we map the Bloch wave-functions onto Wannier orbitals with $d_{x^2-y^2}$ character. The resulting tight-binding model forms a basis for the Hubbard Hamiltonian, which we investigate using the Variational Cluster Approximation.
[1] C.-W. Chen *et al.*, "Orbital selective Mott transition in layered $Sr_2Mn_3As_2O_2$ single crystals" (under review)

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