Abstract Submitted
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**Electronic structure and excitation spectra of transition metal monoxides investigated via orbital-dependent functionals**[1] J. ASHLEY ALFORD, OSCAR D. RESTREPO, ADOLFO G. EGUILUZ, Oak Ridge National Laboratory/Univ. of Tennessee, THOMAS C. SCHULTHESS, Oak Ridge National Laboratory — We are investigating the electronic structure of strongly correlated 3d transition metal monoxides with two orbital dependent functionals, the self-interaction corrected local spin-density method (SIC-LSD) as well as the LDA+U method. Both functionals are known to reproduce the antiferromagnetic insulating ground state of, for example, CoO and NiO. We perform a detailed comparison of magnetic moments, exchange, and electronic structure calculated with the two methods. In addition, we study the interplay between the electronic structure and the electron-hole excitations in both the insulating and the metallic phases. Our results are compared with available experimental data.

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J. Ashley Alford
Oak Ridge National Laboratory/ Univ. of Tennessee

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