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Electronic Structure, Magnetism, and Correlation Effects in Oxychalcogenide $La_2O_2Fe_2OSe_2$ JIAN-XIN ZHU, Los Alamos National Laboratory, RONG YU, Rice University, HANGDONG WANG, Zhejiang University, M. JONES, University at Buffalo, SUNY , JIANHUI DAI, Zhejiang University, E. ABRAHAMS, Rutgers University, MINGHU FANG, Zhejiang University, QIMIAO SI, Rice University — Iron pnictides are the first non-copper-based compounds to exhibit high-T_c superconductivity, and have therefore attracted intense interest. Whether these compounds are weakly interacting metals or bad metals near a Mott transition is a subject of extensive current discussion. Here we consider compounds containing Fe_2O square planar layers. The Fe-Fe distance in these systems is larger than that of their FeAs counterparts, suggesting the possibility of stronger correlation effects. We report the first-principles density functional theory (DFT) calculations on the oxychalcogenides $La_2O_2Fe_2OSe_2$. We have calculated the band structure and compared the results with those of the LaOFeAs compound. We have also extracted, within the GGA+U approximation, the spin exchange interactions. The corresponding frustrated Heisenberg model yields a checkerboard magnetic order, which is consistent with the energetic consideration in the DFT. Finally we discuss these results in light of the experimental data from thermodynamic, transport and neutron scattering measurements.

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