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Anomalous Dynamics of K Ion in β-Pyrochlore JAN KUNES, University of California Davis, TAE SEONG JEONG, WARREN E. PICKETT — Among the recently discovered β-pyrochlore superconductors AOs_2O_6 (A=K, Rb, and Cs) KOs_2O_6 exhibits several anomalous features (electrical resistivity, $1/T_1$ NMR decay). We have studied electronic structure of AOs_2O_6 using the density functional theory based methods. We have found a moderate Stoner enhancement of the Pauli susceptibility of 2.15 and a sizable thermal mass enhancement of 2.9 in KOs_2O_6. While the electronic structure of the three systems is very similar the structural stability of the alkali atom site is rather different. In particular the K ion potential well has a flat bottom, beyond small anharmonic corrections, allowing for large excursions from the symmetric position. We suggest that this feature is behind the striking differences in behavior of otherwise similar AOs_2O_6 compounds.

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