Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic structure properties and superconductivity of the β-pyrochlore Os oxides, $A\mathbf{Os_2O_6}$ (A=alkali metal)[1] R. SANIZ, A. J. FREEMAN, Northwestern U. — The recently discovered[2] family of superconducting β-pyrochlores $A\mathrm{Os_2O_6}$ (A=alkali metal) represents a particularly interesting example of the interplay between superconductivity and orbital and crystal structure degrees of freedom. Indeed, the pyrochlore lattice formed by the Os-O staggered chains appears to lead to very high Sommerfeld coefficients, increasing of T_c under positive pressure, and other intriguing properties. We present results of a first-principles study of the electronic structure and superconducting properties of these materials (A=Na, K, Rb, and Cs) using the highly precise full-potential linearized augmented plane wave (FLAPW) method.[3] We show that the observed increase of T_c with decreasing mass of A as well as under positive hydrostatic pressure can both be well understood within a conventional phonon-mediated pairing picture. Furthermore, the density of states at E_F depends critically on spin-orbit coupling, due to a van Hove singularity near E_F, with a direct effect on T_c; the Fermi surface shows strong nesting, which is reflected in the dynamic susceptibility and thus indicates that spin fluctuations may play an important role in these materials.

[1]Supported by the DOE (grant No. DE-FG02-88ER 45372).
[2]T. Muramatsu *et al.* J. Phys. Soc. Jpn. **73**, 10 (2004).
[3]Wimmer, Krakauer, Weinert, Freeman, Phys. Rev. B **24**, 864 (1981).

R. Saniz
Northwestern U.

Date submitted: 18 Nov 2004 Electronic form version 1.4