First-principles study on the magnetism and metal-insulator transition in pyrochlore oxide $Cd_2Os_2O_7$

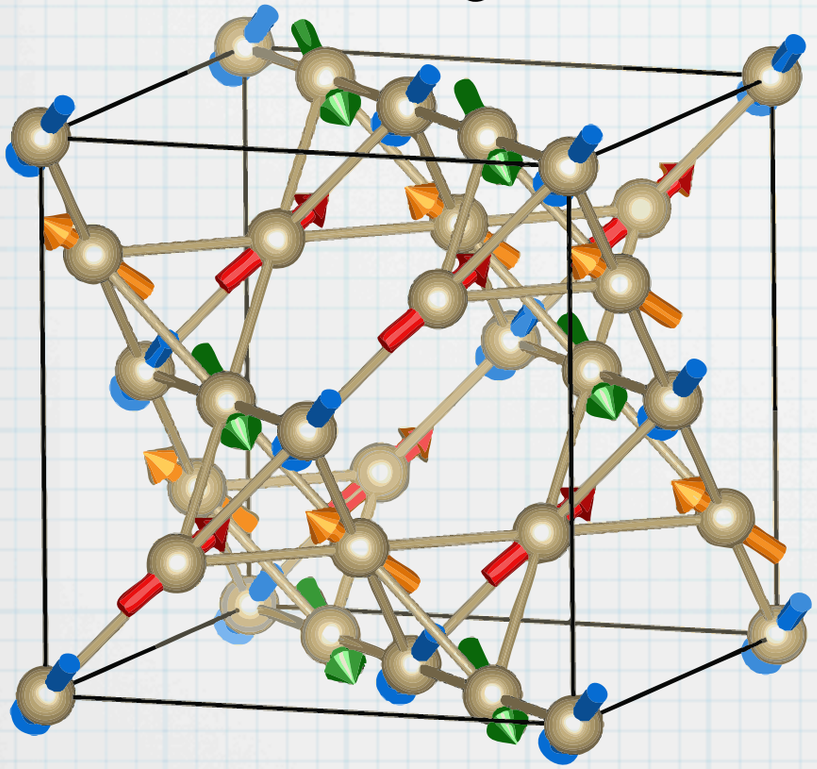
AIST[A], JST-CREST[B]
Hiroshi Shinaoka[A,B], Takashi Miyake[A,B], and Shoji Ishibashi[A]

$Cd_2Os_2O_7$

- 5*d* pyrochlore oxide with long history of study since 1974
- Metal-insulator transition at 227 K
- Néel-type ordering of Os spins at low *T*

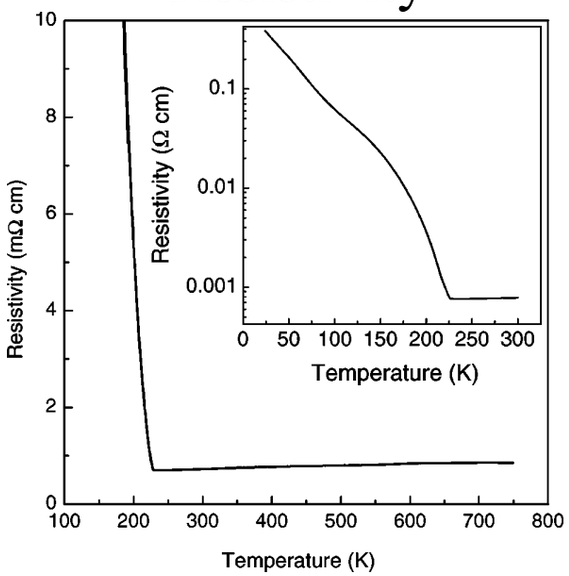
Os^{5+} ($5d^3$) *cf.* Ir^{4+} ($5d^5$, J_{eff}=1/2)

All-in/all-out magnetic order



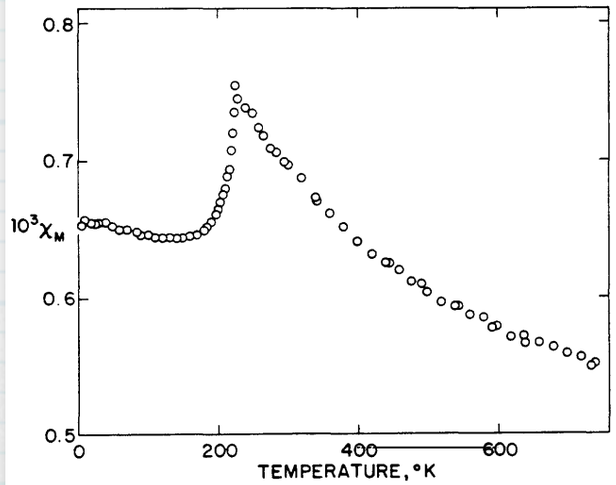
Corner-sharing tetrahedral "pyrochlore" network of Os

Resistivity



D. Mandrus *et al*., Rev. **B** 63, 195104 (2001)

Magnetic susceptivity

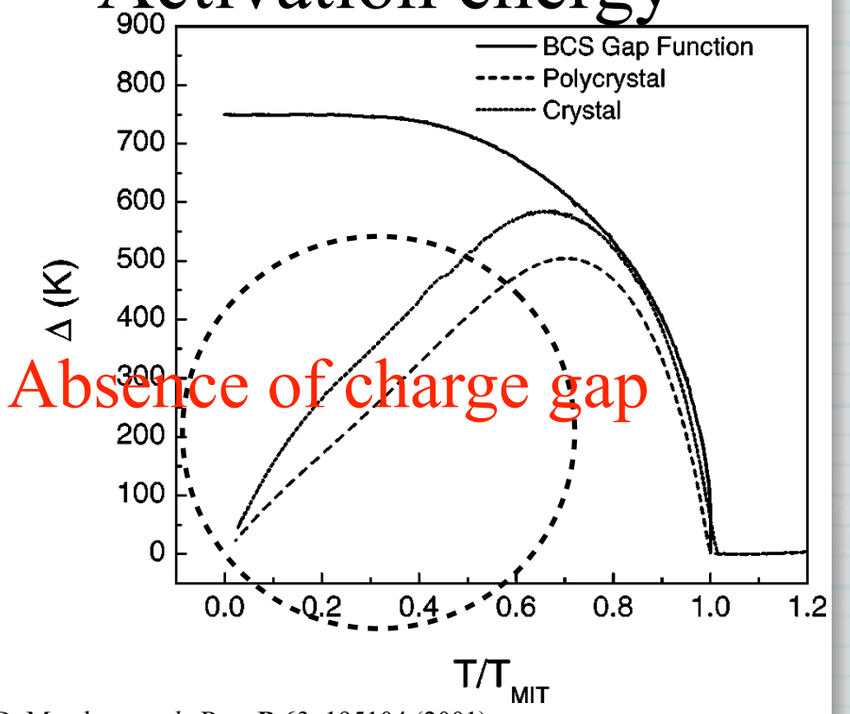


A. Sleight *et al*., Solid State Comm. **14**, 357 (1974)

Recently, the all-in/all-out magnetic ordering was suggested by X-ray experiments (Yamaura *et al*.) and NMR experiments (Yamauchi *et al*.).

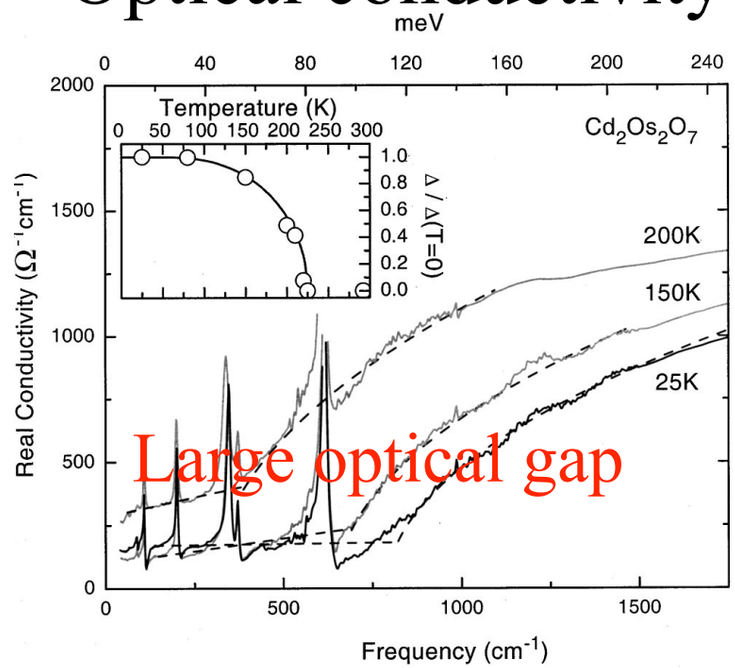
Peculiar properties of $Cd_2Os_2O_7$

Activation energy



D. Mandrus *et al.*, Rev. **B** 63, 195104 (2001)

Optical conductivity



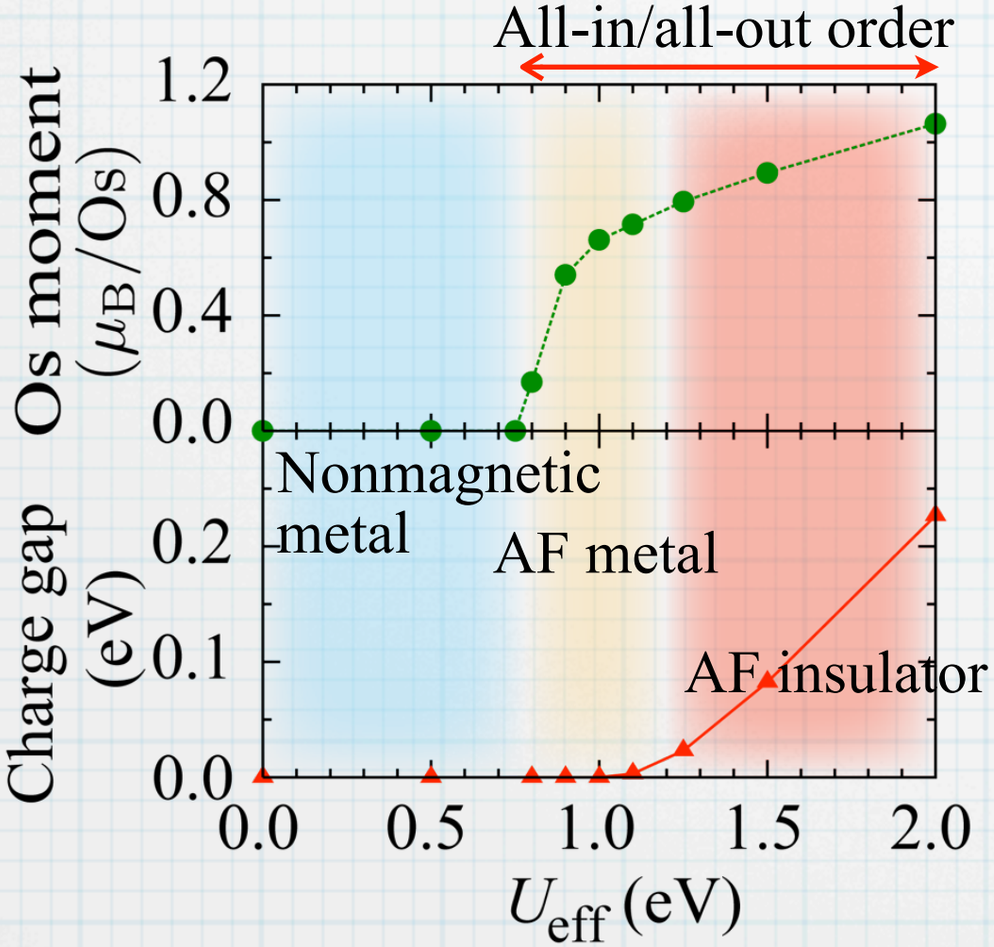
- Absence of a clear charge gap vs. the opening of an optical gap
- Semiconducting behavior up to high *T*
- The *highest* transition temperature among magnetic pyrochlore oxides

So far, no first-principles study is available concerning electronic properties of the magnetic ground state.

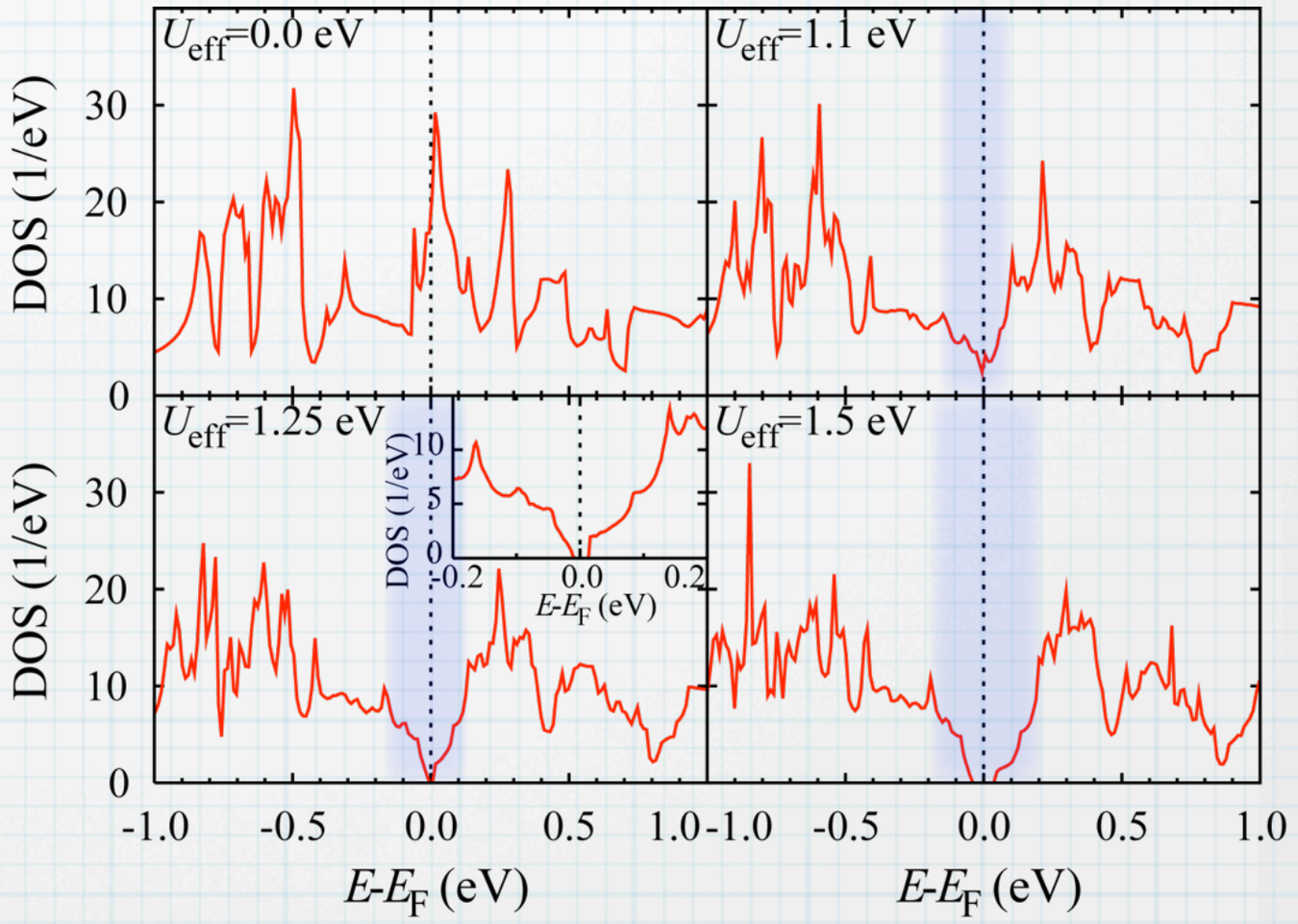
Results

- LSDA+SO+U $\quad U_{\mathrm{eff}} \equiv U - J$
- PAW computational code: Quantum MAterials Simulator (QMAS)

Phase diagram



Density of states



- All-in/all-out order is stabilized by strong easy-axis anisotropy (~50 meV)
- Semi-metallic band structure / *pseudo gap* near MIT

→Calculated results well explain the peculiar low-T characteristics