

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Electronic structure of lead pyrophosphate** MALLIGA SUEWATTANA, DAVID SINGH, Oak Ridge National Laboratory — Lead Pyrophosphate  $\text{Pb}_2\text{P}_2\text{O}_7$  is of interest for potential radiation detection applications and use in long term waste storage. It forms in triclinic  $\text{P}\bar{1}$  crystals and can also be grown as glasses. We performed electronic structure calculations using the crystal structure which determined by Mullica et. al (J. Solid State Chem (1986)) using x-ray diffraction and found large forces on atoms suggesting that the refined atomic positions were not fully correct. Here we report first principles structure relaxation and a revised crystal structure for this compound. We analyze the resulting structure using pair distribution functions and discuss the implications for the electronic properties. This work was supported by DOE NA22 and the Office of Naval Research.

Malliga Suewattana  
Oak Ridge National Laboratory

Date submitted: 15 Nov 2006

Electronic form version 1.4