Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Comparison of the electronic structures of four crystalline forms of $FePO_4$.[1] PING TANG, N. A. W. HOLZWARTH, Wake Forest University — The purpose of this study is to investigate the stability of $FePO_4$, the fully charged form of the Li ion battery material, $LiFePO_4$. The electronic structures of four phases of $FePO_4$, having the $CrVO_4$,[2] quartz,[3] monoclinic,[4] and olivine[5] structures are studied using density functional theory with LSDA and GGA exchange-correlation functionals. A ferromagnetic spin configuration is chosen for all of the $FePO_4$ calculations. The band structures, density of states, and total energies are compared among all four phases. The results show that the $CrVO_4$ phase is metallic while the other phases are insulating. The band gaps of the insulating phases are found to increase with decreasing density of the material.

[1]Supported by NSF Grant No. DMR-0405456.
[2]J. P. Attfield and co-workers, *J. Solid State Chem.* **57**, 357 (1985)
[3]H. N. Ng and C. Calvo, *Can. J. Chem.* **53**, 2064 (1975)
[4]Y. Song and co-workers, *Inorg. Chem.* **41**, 5778 (2002)
[5]A. S. Andersson and co-workers, *Solid State Ionics* **130**, 41 (2000)

N. A. W. Holzwarth
Wake Forest University

Date submitted: 30 Nov 2004 Electronic form version 1.4