Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Comparison of the electronic structures of four crystalline phases of $FePO_4$[1] PING TANG, N. A. W. HOLZWARTH, Wake Forest University — $LiFePO_4$ in the olivine structure is a promising cathode material for Li-ion batteries. During normal battery operation, an olivine form of $FePO_4$ is formed. Experimental evidence suggests that the olivine phase is meta-stable relative to a quartz-like trigonal phase. In addition, several other meta-stable phases have been reported[2] including a monoclinic and a high pressure $CrVO_4$ structure. We have carried first-principles electronic structure calculations on all of these phases in order to investigate their relative stability and other properties using both LAPW and PWPAW methods.[3] We find that the LSDA approximation systematically underestimates the lattice constants and the calculated stability ordering of the phases is inconsistent with experiment. In contrast the GGA approximation models the phase stability in closer agreement with experiment, although the lattice constants are systematically over-estimated.

[1]Supported by NSF Grant No. DMR-0405456.
[2]M. S. Whittingham, Chem. Rev. **104**, 4271 (2004); Y. Song and co-workers, Inorg. Chem. **41**, 5778 (2002); H. N. Ng and C. Calvo, Can. J. Chem. **53**, 2064 (1975); J. P. Attfield and co-workers, J. Solid State Chem. **57**, 357 (1985); A. S. Andersson and co-workers, Solid State Ionics **130**, 41 (2000)
[3]http://www.wien2k.at/; http://pwpaw.wfu.edu/

Natalie Holzwarth
Wake Forest University

Date submitted: 02 Dec 2005 Electronic form version 1.4