Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Correlating cation coordination, stiffness, phase transition pressures, and smart materials behavior in metal phosphates DMITRY SHAKHVOROSTOV, University of Western Ontario, NICHOLAS MOSEY, University of Kingston, YANG SONG, PETER NORTON, MARTIN MUESER, University of Western Ontario — In this study, we present X-ray diffraction data on zinc- and calcium phosphates. The experiments reveal that low-coordinated zinc phosphates are relatively soft at ambient conditions but stiffen dramatically with pressure, p, exhibiting smart materials behavior, while high-coordinated zinc and calcium phosphates have higher initial bulk moduli and stiffen considerably less rapidly with increasing p. All systems amorphize when their bulk modulus reaches a value near 210 ± 40 GPa, where the precise value depends on chemical details, indicating that phosphate networks become unstable when their bulk modulus reaches that value. Our ab initio simulations of zinc α-phosphate support the idea that the elastic properties are controlled by the motion of rigid phosphate units, which becomes more hindered under densification, with or without increasing cation coordination. It is discussed how these results may explain why low-coordinated zinc phosphates are good anti-wear agents.

Dmitry Shakhvorostov
University of Western Ontario

Date submitted: 19 Nov 2008 Electronic form version 1.4