Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Electronic structure and the suppression of the Jahn-Teller distortion in the quantum antiferromagnet $Ba_3CuSb_2O_9$ K.V. SHANAVAS, Z. POPOVIC, S. SATPATHY, Department of Physics & Astronomy, University of Missouri — In recent years, the field of geometrically frustrated materials have regained interest by the dicsovery of several candidates for quantum spin liquids. The antiferromagnet $Ba_3CuSb_2O_9$ is one such material where the $S = \frac{1}{2}$ on a triangular (more recently hexagonal) lattice leads to frustration. Using density functional methods, we study the electronic structure of the material, both in the triangular lattice as well as the honeycomb structure. For both structures, a simple tight-binding description involving the Cu (e_g) orbitals describes the band structure rather well, confirming the central role of these orbitals in the physics of the problem. It has been suggested that the Jahn-Teller effect could play an important role in the properties of the system. We find that in spite of the presence of the Cu (d^9) ion, the Jahn-Teller coupling is surprisingly weak in the material, which suppresses any Jahn-Teller distortion of the CuO_9 octahedra in the compound.

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Date submitted: 17 Nov 2012 Electronic form version 1.4